Bosons in Jellium

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Le coeur a ses raisons, que la raison
ne connaît point; on le sait en mille choses.

Blaise Pascal (1623-1662),
Pensées 477 (uitgave J. Chevalier)

Voor mijn ouders

Voor Yolande

VOORWOORD

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Contents

INTRODUCTION

The jellium model consists of interacting electrons moving against a uniform background of neutralizing positive charge. It is thought relevant for an understanding of the behaviour of electrons in metals. Exact solutions of the jellium model are only known in the limits of very low and very high electron density. In both limits the exact ground state energy of the jellium model can be obtained by reformulating the model in terms of bosons. The existing boson formulations, however, give rise to some fundamental questions.

In the limit of low density the existing boson formulation, which is due to Carr [1], is based upon a semi-classical approach. As a consequence Carr's Hamiltonian is not invariant under the permutation of the coordinates of the electrons, its ground state is not antisymmetric and the relation between the introduced bosons and the original fermions is unclear.

In the high-density limit the existing boson formulation, which is due to Sawada [2], is based upon perturbation theory with the Sommerfeld free-electron model as the unperturbed system. Sawada's formulation is an elegant way to avoid the problem of the so-called infrared divergency, that appears in second order perturbation theory due to the long-range nature of the Coulomb interaction. As a consequence of the perturbational approach, however, Sawada's boson Hamiltonian does not take into account the full dynamics of the fermion system, i.e. its meaning is unclear.

This thesis discusses the fundamental questions raised by the existing boson formulations and presents different boson formulations. In part I the semi-classical approach to the low-density jellium model is replaced by a fully quantummechanical treatment. The resulting boson formulation is used to study the effect of a magnetic field on the jellium model. In part II the algorithm is given for the construction of a boson Hamiltonian, that includes the full description of the jellium model at all densities. This algorithm is applied to a reduced form of the jellium model, that has the same ground state energy as the jellium model in the high-density limit.

References

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I Quantum field approach to a low-density electron system *

Abstract

The semi-classical approach to an interacting electron system with low density is replaced by a fully quantummechanical discussion. The energies of the ground state and the low lying excited states are calculated according to the methods of quantum field theory. A comparison is made with the results of the existing approach. The effect of a magnetic field on the low lying states of the electron system is calculated in a selfconsistent way. The low density electron system does not show a Meissner-Ochsenfeld effect.

1. Introduction

The jellium model plays a prominent part in our understanding of the behaviour of the solid state. This model consists of a number of interacting electrons that move against a uniform background of neutralizing positive charge. Up to now its exact solution is unknown and one has to resort to approximation methods in order to study its behaviour. According to Wigner [1], who used a semi-classical approach, the ground state of the jellium model has a lattice structure at sufficiently low densities. This electron lattice is known as the Wigner lattice. For a review of the existing literature on the Wigner lattice we refer to Care and March [2].

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The aim of the present article is to discuss the properties of the ground state and the low lying excited states of the low density jellium model from a purely quantummechanical point of view. Our paper is organized in the following way. First, in section 2, we discuss briefly the formation of a lattice structure in the classical jellium model. Next, in section 3, we give a rather elaborated discussion of the ground state using a quantum field approach. Our calculations are based on the variational method using a Hartree-Fock trial state. Most of the results are familiar, but they are now based on a fully quantummechanical ground. In section 4 we consider the influence of correlation on the Hartree-Fock results. Section 5 deals with the effect of a magnetic field on the Wigner lattice and pays attention to the eventual appearance of superconductivity. Finally the results are discussed in section 6.

2. Lattice formation in the classical jellium model

First of all we recall briefly the jellium model. The starting-point of our discussion is a system that consists of N electrons and N positive ions moving in a volume Ω. The Hamiltonian of this system is given by

$$H = \sum_k (\frac{\boldsymbol{p}_k^2}{2m} + \frac{\boldsymbol{\pi}_k^2}{2M}) + \frac{1}{2} e^2 \sum_{k \neq l} (\frac{1}{|\boldsymbol{r}_k - \boldsymbol{r}_l|} + \frac{1}{|\boldsymbol{\rho}_k - \boldsymbol{\rho}_l|}) - e^2 \sum_{k,l} \frac{1}{|\boldsymbol{r}_k - \boldsymbol{\rho}_l|}, \qquad (2.1)$$

where e is the magnitude of the charge of an electron or ion, m the mass of an electron, M the mass of an ion, whereas $\boldsymbol{r}_k$ and $\boldsymbol{p}_k$ denote the position and momentum of electron k and $\boldsymbol{\rho}_k$ and $\boldsymbol{\pi}_k$ those of ion k. Next we use the decomposition

$$\frac{e^2}{r} = \sum_{\boldsymbol{q}} V(\boldsymbol{q}) \exp(i\boldsymbol{q} \cdot \boldsymbol{r}) \equiv \frac{\Omega}{(2\pi)^3} \int d^3q\, V(\boldsymbol{q}) \exp(i\boldsymbol{q} \cdot \boldsymbol{r}) \qquad (2.2)$$

with

$$V(\boldsymbol{q}) = \frac{1}{\Omega} \int d^3r \frac{e^2}{r} \exp(-i\boldsymbol{q} \cdot \boldsymbol{r}) = \frac{4\pi e^2}{\Omega q^2}. \qquad (2.3)$$

It should be remarked here that strictly speaking the expression (2.3) is only true if the Coulomb potential $\frac{1}{r}$ is replaced by the Yukawa potential $\frac{e^{-\mu r}}{r}$ and the limit $\mu \to 0$ is taken after performing the integration. Substitution of (2.2) into (2.1) gives

$$\begin{aligned} H &= \sum_k (\frac{\boldsymbol{p}_k^2}{2m} + \frac{\boldsymbol{\pi}_k^2}{2M}) + \frac{1}{2} {\sum_{\boldsymbol{q}}}' V(\boldsymbol{q}) \Bigg[\sum_{k \neq l} (\exp[i\boldsymbol{q} \cdot (\boldsymbol{r}_k - \boldsymbol{r}_l)] \\ &+ \exp[i\boldsymbol{q} \cdot (\boldsymbol{\rho}_k - \boldsymbol{\rho}_l)]) - 2 \sum_{k,l} \exp[i\boldsymbol{q} \cdot (\boldsymbol{r}_k - \boldsymbol{\rho}_l)] \Bigg] - NV(0), \qquad (2.4) \end{aligned}$$

where the prime in the summation over $\boldsymbol{q}$ indicates that the $\boldsymbol{q} = 0$ term is excluded. The term $NV(0)$ does not contribute to the energy per electron in the thermodynamic limit, as follows from the integral representation (2.3). Consequently this term can be neglected. The jellium model is then obtained by putting the momenta of the ions equal to zero and by averaging the Hamiltonian (2.4) over all possible configurations of the ions attributing equal weight to them. The result is a homogeneous positively charged background for the electrons. The Hamiltonian of the jellium model is

$$H = \sum_k \frac{\boldsymbol{p}_k^2}{2m} + \frac{1}{2} {\sum_{\boldsymbol{q}}}' V(\boldsymbol{q}) \sum_{k \neq l} \exp[i\boldsymbol{q} \cdot (\boldsymbol{r}_k - \boldsymbol{r}_l)]. \qquad (2.5)$$

Here we pay attention to the energy of the ground state of the classical jellium model. This means that the momenta of the electrons are zero and that we must look for a distribution function $\Phi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N)$ that minimizes the energy expression

$$E = \frac{1}{2} {\sum_{\boldsymbol{q}}}' V(\boldsymbol{q}) \int d^3r_1 \ldots d^3r_N \, \Phi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N) \sum_{k \neq l} \exp[i\boldsymbol{q} \cdot (\boldsymbol{r}_k - \boldsymbol{r}_l)] , \tag{2.6}$$

where Φ is normalized, i.e.

$$\int d^3r_1 \ldots d^3r_N \, \Phi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N) = 1 . \tag{2.7}$$

As discussed by Peierls [3] a regular lattice of electrons is expected to be the most stable configuration. Denoting the lattice positions by the set $\{\boldsymbol{R}_k | k = 1, \ldots, N\}$ and putting

$$\Phi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N) = \prod_{k=1}^{N} \delta^3(\boldsymbol{r}_k - \boldsymbol{R}_k) \tag{2.8}$$

we obtain using (2.3)

$$E = \frac{2\pi e^2}{\Omega} {\sum_{\boldsymbol{q}}}' \sum_{k \neq l} \frac{1}{q^2} \exp[i\boldsymbol{q} \cdot (\boldsymbol{R}_k - \boldsymbol{R}_l)] . \tag{2.9}$$

The expression (2.9) contains a summation over the lattice points, which can be easily performed. Then the energy per electron, $\varepsilon = \frac{E}{N}$, appears to be

$$\begin{aligned} \varepsilon &= \frac{2\pi e^2}{N\Omega} {\sum_{\boldsymbol{q}}}' \frac{1}{q^2} \Big(\sum_{k,l} \exp[i\boldsymbol{q} \cdot (\boldsymbol{R}_k - \boldsymbol{R}_l)] - N \Big) \\ &= \frac{2\pi e^2}{\Omega} \Big({\sum_{\boldsymbol{K}_n}}' \frac{N}{K_n^2} - {\sum_{\boldsymbol{q}}}' \frac{1}{q^2} \Big) , \end{aligned} \tag{2.10}$$

where $\boldsymbol{K}_n$ denotes a reciprocal lattice vector. The energy ε is negative for all electron densities, as the primitive unit cell of the reciprocal lattice contains N $\boldsymbol{q}$ points. Clearly expression (2.10) consists of two divergent terms. However, their difference is finite as can be shown using the Madelung or Ewald summation procedure. For several lattices the energy ε has been calculated, see e.g. Sholl [4]. It appears that the body-centered cubic lattice has the lowest energy, but it should be remarked here that the energy difference with other simple lattice structures is extremely small.

Summarizing we can conclude that the ground state of the classical jellium model is a b.c.c.-lattice for all electron densities.

3. Hartree-Fock ground state of the quantummechanical low-density jellium model

The Hamiltonian of the quantummechanical version of the jellium model (2.5) reads in the formalism of second quantization

$$H = \sum_{\boldsymbol{k},\sigma} \frac{\hbar^2 k^2}{2m} c^+_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + \frac{1}{2} \sum_{\substack{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q} \\ \sigma,\sigma'}}{}' V(\boldsymbol{q})\, c^+_{\boldsymbol{k}\sigma}\, c^+_{\boldsymbol{k}'\sigma'}\, c_{\boldsymbol{k}'+\boldsymbol{q}\sigma'}\, c_{\boldsymbol{k}-\boldsymbol{q}\sigma} \,, \tag{3.1}$$

where the fermion operators $c^+_{\boldsymbol{k}\sigma}$ and $c_{\boldsymbol{k}\sigma}$ create and annihilate respectively an electron in a plane wave state labeled by the wave vector $\boldsymbol{k}$ and spin σ. The prime in the summation indicates that the $\boldsymbol{q} = 0$ term is excluded because of the presence of the homogeneous positively charged background.

Consider a system consisting of $2N$ electrons, where the number $2N$ has been chosen for convenience. The ground state of the jellium model can be expressed as

$$|\Psi\rangle = \sum_{\sigma_1,\ldots,\sigma_{2N}} \int d^3r_1 \ldots d^3r_{2N}\, F(\boldsymbol{r}_1,\sigma_1;\ldots;\boldsymbol{r}_{2N},\sigma_{2N}) \psi^+_{\sigma_1}(\boldsymbol{r}_1)\ldots\psi^+_{\sigma_{2N}}(\boldsymbol{r}_{2N})|\rangle \,, \tag{3.2}$$

where $|\rangle$ denotes the vacuum state and $\psi^+_\sigma(\boldsymbol{r})$ is the usual field operator creating a fermion with spin σ at the position $\boldsymbol{r}$,

$$\psi^+_\sigma(\boldsymbol{r}) = \frac{1}{\sqrt{\Omega}} \sum_{\boldsymbol{k}} \exp(-i\boldsymbol{k}\cdot\boldsymbol{r})\, c^+_{\boldsymbol{k}\sigma} \,. \tag{3.3}$$

The function F is determined by the requirement that it must minimize the energy of the system, i.e. the expression

$$E = \langle\Psi|H|\Psi\rangle \,. \tag{3.4}$$

It should be remarked here that F is not the Schrödinger representation of the ground state of the system. That wave function is obtained by constructing the antisymmetrized form of the original function F. The quantity $|F|^2$ plays a similar role as the classical distribution function Φ.

In practice the exact calculation of the ground state energy is still an insurmountable problem. Therefore, one has to resort to approximation methods. Here we have chosen the variational method because of her elegant and insight providing character. In this section we consider the simplest Ansatz for F, namely the so-called Hartree-Fock (HF) approximation, i.e.

$$F(\boldsymbol{r}_1, \sigma_1; \ldots; \boldsymbol{r}_{2N}, \sigma_{2N}) = C \prod_{n=1}^{2N} f_n(\boldsymbol{r}_n, \sigma_n) \;, \tag{3.5}$$

where the function f_n represents a normalized one-particle wave function, and C is the normalization constant for $|\Psi\rangle$. Next we recall that the ground state of the classical system is a b.c.c.-lattice. Such a structure can also be expected in the quantummechanical analogue provided that the one-particle wave functions are localized but such that their attendant kinetic energies are small. That requirement can only be fulfilled for an electron system of sufficiently low density. Therefore we restrict ourselves to the low-density jellium model. The translational invariance of the supposed lattice structure implies

$$f_n(\boldsymbol{r}_n, \sigma_n) = f(\boldsymbol{r}_n - \boldsymbol{R}_n)\, \delta_{\sigma_n \tau_n} \;, \tag{3.6}$$

with $\boldsymbol{R}_n$ being a lattice vector and τ_n the spin of the particle localized at $\boldsymbol{R}_n$. Substitution of (3.5) into (3.2) and making use of (3.6) gives us the following HF trial state as an approximation of the ground state of the low-density jellium model:

$$|\Psi_{HF}\rangle = C\, d^+_{\tau_1}(\boldsymbol{R}_1) \ldots d^+_{\tau_{2N}}(\boldsymbol{R}_{2N})|\rangle \;, \tag{3.7}$$

where the operator $d^+_{\tau_n}(\boldsymbol{R}_n)$ describes the creation of an electron with spin τ_n in the wave function f localized around the lattice point $\boldsymbol{R}_n$:

$$d^+_{\tau_n}(\boldsymbol{R}_n) = \int d^3r\, \psi^+_{\tau_n}(\boldsymbol{r}) f(\boldsymbol{r} - \boldsymbol{R}_n) \;. \tag{3.8}$$

Representing the wave function as the Fourier integral

$$f(\boldsymbol{r}) = \frac{1}{(2\pi)^{3/2}} \int d^3k\, \hat{f}(\boldsymbol{k}) \exp(\imath \boldsymbol{k} \cdot \boldsymbol{r}) \tag{3.9}$$

with

$$\hat{f}(\boldsymbol{k}) = \frac{1}{(2\pi)^{3/2}} \int d^3r\, f(\boldsymbol{r}) \exp(-\imath \boldsymbol{k} \cdot \boldsymbol{r}) \tag{3.10}$$

the creation operator (3.8) can be expressed as

$$d^{+}_{\tau_n}(\boldsymbol{R}_n) = \left[\frac{(2\pi)^3}{\Omega}\right]^{\frac{1}{2}} \sum_{\boldsymbol{k}} \exp(-\imath \boldsymbol{k}\cdot\boldsymbol{R}_n)\hat{f}(\boldsymbol{k})\, c^{+}_{\boldsymbol{k}\tau_n} \ . \tag{3.11}$$

It follows immediately from (3.8) that the newly defined creation and annihilation operators satisfy the following anticommutation relations

$$\begin{aligned} \left\{d_{\tau_m}(\boldsymbol{R}_m), d^{+}_{\tau_n}(\boldsymbol{R}_n)\right\} &= \delta_{\tau_m\tau_n} S(\boldsymbol{R}_m - \boldsymbol{R}_n), \\ \{d_{\tau_m}(\boldsymbol{R}_m), d_{\tau_n}(\boldsymbol{R}_n)\} &= \left\{d^{+}_{\tau_m}(\boldsymbol{R}_m), d^{+}_{\tau_n}(\boldsymbol{R}_n)\right\} = 0 \ , \end{aligned} \tag{3.12}$$

where

$$S(\boldsymbol{R}_m - \boldsymbol{R}_n) = \int d^3r\, f^{*}(\boldsymbol{r} - \boldsymbol{R}_m) f(\boldsymbol{r} - \boldsymbol{R}_n) \ . \tag{3.13}$$

The quantity $S(\boldsymbol{R}_m - \boldsymbol{R}_n)$ is the overlap of two wave functions centered around $\boldsymbol{R}_m$ and $\boldsymbol{R}_n$ respectively.

In a first approximation the overlap between the distinct wave functions can be neglected. Then the energy appears to be independent of the spin configuration as shown in Appendix I. The resulting energy, which is a functional of the wave function f, is just the Hartree energy

$$E_H(f) = 2N \int d^3k\, \frac{\hbar^2 k^2}{2m}\, \hat{f}(\boldsymbol{k})\hat{f}^{*}(\boldsymbol{k}) + \frac{1}{2} {\sum_{\boldsymbol{q}}}' \sum_{m\neq n} \tilde{V}(\boldsymbol{q}\,) \exp[\imath \boldsymbol{q}\cdot(\boldsymbol{R}_n - \boldsymbol{R}_m)] \ , \tag{3.14}$$

where

$$\tilde{V}(\boldsymbol{q}\,) = V(\boldsymbol{q}\,) \left[\int d^3k\, \hat{f}(\boldsymbol{k}+\boldsymbol{q}\,)\hat{f}^{*}(\boldsymbol{k})\right]^2 \ . \tag{3.15}$$

N.B. It should be stressed here that the expression for the Hartree energy still contains terms of the order of the overlap. These terms do not originate from the presence of $S(\boldsymbol{R}_m - \boldsymbol{R}_n)$ in the anticommutation relations (3.12) but are due to the form of $\tilde{V}(\boldsymbol{q}\,)$ given by (3.15). Clearly $\tilde{V}(\boldsymbol{q}\,)$ is not the Fourier transform of the Coulomb potential but of some smeared-out potential that depends on the wave function f itself.

The explicit form of the wave function f follows from the condition that f must minimize $E_H(f)$. That minimization procedure is discussed in Appendix II. It appears

that the resulting form is given by

$$f_0(\boldsymbol{r}) = \frac{1}{(2\alpha\pi)^{3/4}} \exp\left(-\frac{r^2}{4\alpha}\right) \tag{3.16}$$

with

$$\alpha^2 = \frac{3\Omega}{32\pi N} \frac{\hbar^2}{me^2} , \tag{3.17}$$

provided that all terms of the order of the overlap are neglected. The attendant Hartree energy is

$$E_H^{(0)} = E_{Cl} + 2N \frac{8\pi N e^2 \alpha}{\Omega} , \tag{3.18}$$

where E_{Cl} denotes the energy of the classical electron lattice. We like to remark here that $E_H^{(0)}$ is not the energy obtained by substituting (3.16) into (3.14), the difference being of the order of the overlap.

In order to compare our results with existing ones we use the Bohr unit $a_0 = \frac{\hbar^2}{me^2}$ as the unit of length and the Rydberg, which equals $\frac{e^2}{2a_0}$, as the unit of energy. Further we express the electron density ρ in terms of the dimensionless parameter r_s according to:

$$\rho = \frac{2N}{\Omega} = \left(\frac{4}{3}\pi r_s^3 a_0^3\right)^{-1} . \tag{3.19}$$

Then the following expressions are obtained for α and $E_H^{(0)}$ respectively:

$$\alpha = \frac{1}{2} r_s^{3/2} a_0^2 , \tag{3.20}$$

$$E_H^{(0)} = 2N \left(-\frac{A}{r_s} + \frac{3}{r_s^{3/2}}\right) , \tag{3.21}$$

where A is the Madelung constant of the classical electron lattice.

The overlap (3.13) can be easily calculated for a wave function of the form (3.16) and appears to be

$$S(\boldsymbol{R}_{mn}) = \exp\left(-\frac{R_{mn}^2}{8\alpha}\right) = \exp\left(-\frac{1}{4}\tilde{R}_{mn}^2 r_s^{1/2}\right) \tag{3.22}$$

with $|\boldsymbol{R}_m - \boldsymbol{R}_n| = |\boldsymbol{R}_{mn}| = R_{mn}$ and $\tilde{R}_{mn} = \frac{R_{mn}}{r_s a_0}$, i.e. $\tilde{R}_{mn}$ is a dimensionless measure for the distance between the lattice positions $\boldsymbol{R}_m$ and $\boldsymbol{R}_n$. The quantity $\tilde{R}_{mn}$ is of the order of one or larger as the lattice distance is of the order of $r_s a_0$. Consequently the overlap is very small indeed at low density, i.e. for large r_s.

Our results (3.20) and (3.21) are exactly equal to those of Wigner, i.e. the Wigner treatment is equivalent to an approximate Hartree-Fock calculation based on localized one-electron wave functions. The approximation consists of neglecting the mutual overlap (3.22) of the wave functions in the anticommutation relations (3.12) plus all terms in the resulting Hartree energy, which are of the same order as the overlap.

The difference between the Hartree-Fock energy and the Hartree energy is known as the exchange energy and depends on the spin configuration of the underlying lattice. In the following we discuss the Hartree-Fock energy up to order $S(\boldsymbol{R}_{mn})^2$ for both the ferromagnetic and the antiferromagnetic spin configuration. The overlap terms of order $S(\boldsymbol{R}_{mn})^2$ are two-particle exchange terms. These terms have also been discussed by Carr [5]. Higher order corrections to the Wigner energy (3.21) are not considered here because of the complexity of the calculations.

As shown in Appendix II the wave function, that minimizes the Hartree-Fock energy E_{HF} up to order $S(\boldsymbol{R}_{mn})^2$, is given by (3.16) plus correction terms of order $S(\boldsymbol{R}_{mn})^2$. The effect of these last terms on E_{HF}, however, is of order $S(\boldsymbol{R}_{mn})^4$ and can therefore be neglected. Thus E_{HF} can be calculated exactly up to order $S(\boldsymbol{R}_{mn})^2$, using the wave function (3.16) with the Wigner α (3.17). The effect of the overlap on the wave function itself is extremely difficult to calculate even up to order $S(\boldsymbol{R}_{mn})^2$. However, that effect can be estimated by choosing the wave function (3.16) as a trial function with variational parameter α and subsequently minimizing the expression for the Hartree-Fock energy up to order $S(\boldsymbol{R}_{mn})^2$ with respect to α. The difference between the resulting value of α and the Wigner value (3.17) is then a measure for the influence of exchange on the wave function.

Up to order $S(\boldsymbol{R}_{mn})^2$ the Hartree-Fock energy consists of two terms. The first term is obtained by substituting (3.16) into (3.14) and performing the lattice sum. It is the total Hartree energy, including all terms of order $S(\boldsymbol{R}_{mn})^2$. The second term is the two-particle exchange energy ΔE_{HF}. The calculation of this energy is given in Appendix I. Thus the

Hartree-Fock energy can be expressed as

$$E_{HF} = 2N\left[\frac{3\hbar^2}{8m\alpha} + N\sum_{\boldsymbol{K}_n\neq 0}\tilde{V}(\boldsymbol{K}_n) - \frac{1}{2}{\sum_{\boldsymbol{q}}}'\tilde{V}(\boldsymbol{q})\right] + \Delta E_{HF}\,, \tag{3.23}$$

where

$$\tilde{V}(\boldsymbol{q}) = \frac{4\pi e^2}{\Omega q^2}\exp(-\alpha q^2) \tag{3.24}$$

and the summation over $\boldsymbol{K}_n$ $(n = 1, 2, \ldots, 2N)$ runs over the reciprocal lattice vectors. The contribution ΔE_{HF} depends on the spin configuration of the Wigner lattice. Here we consider both the purely ferromagnetic configuration and an antiferromagnetic configuration consisting of two interpenetrating sublattices having an oppositely directed purely ferromagnetic spin configuration.

The ferromagnetic two-particle exchange energy is given in expression (I.24) of Appendix I. After performing a simple lattice summation we find

$$\begin{aligned}\Delta E^{f}_{HF} &= 2N\sum_{\boldsymbol{R}_n\neq 0} e^{-R_n^2/4\alpha}\left[\frac{\hbar^2 R_n^2}{32m\alpha^2} + 2N\sum_{\boldsymbol{K}_n\neq 0}\tilde{V}(\boldsymbol{K}_n)[1 - e^{-\frac{1}{2}i\boldsymbol{K}_n\cdot\boldsymbol{R}_n}]\right.\\ &+ \left.{\sum_{\boldsymbol{q}}}'\tilde{V}(\boldsymbol{q})[2\,e^{\frac{1}{2}i\boldsymbol{q}\cdot\boldsymbol{R}_n} - \frac{3}{2} - \frac{1}{2}e^{i\boldsymbol{q}\cdot\boldsymbol{R}_n}]\right]\,,\end{aligned} \tag{3.25}$$

where the summation over $\boldsymbol{R}_n$ $(n = 1, 2, \ldots, 2N)$ runs over the sites of the Wigner lattice, whose reciprocal lattice vectors are denoted by $\boldsymbol{K}_n$. The antiferromagnetic contribution, which is given in (I.25) is found to read, after performing a simple lattice summation

$$\begin{aligned}\Delta E^{a}_{HF} &= 2N\sum_{\boldsymbol{R}_n\neq 0} e^{-R_n^2/4\alpha}\left[\frac{\hbar^2 R_n^2}{32m\alpha^2}\right.\\ &+ N\sum_{\boldsymbol{K}_n\neq 0}\tilde{V}(\boldsymbol{K}_n)[1 + e^{i\boldsymbol{K}_n\cdot\boldsymbol{\delta}}][1 - e^{-\frac{1}{2}i\boldsymbol{K}_n\cdot\boldsymbol{R}_n}]\\ &+ \left.{\sum_{\boldsymbol{q}}}'\tilde{V}(\boldsymbol{q})[2\,e^{\frac{1}{2}i\boldsymbol{q}\cdot\boldsymbol{R}_n} - \frac{3}{2} - \frac{1}{2}e^{i\boldsymbol{q}\cdot\boldsymbol{R}_n}]\right]\,,\end{aligned} \tag{3.26}$$

where the summations over $\boldsymbol{R}_n$ and $\boldsymbol{K}_n$ $(n = 1, 2, \ldots, N)$ now run over the sites of the ferromagnetic sublattice and its reciprocal lattice vectors respectively. The vector $\boldsymbol{\delta}$ describes the position of both sublattices with respect to each other.

For an explicit calculation of the quantities given by (3.23), (3.25) and (3.26) we use the Ewald summation method and replace the Riemann sum over $\boldsymbol{q}$ by an integration. Then we obtain the following expression for the Hartree-Fock energy (see Appendix III):

$$E_{HF} = 2N\left[\frac{3\hbar^2}{8m\alpha}+\frac{4\pi Ne^2}{\Omega}(\alpha-\beta)+\frac{4\pi Ne^2}{\Omega}\sum_{\boldsymbol{K}_n\neq 0}\frac{e^{-\beta K_n^2}}{K_n^2}-\frac{e^2}{2\sqrt{\pi\beta}}\right.$$
$$\left.+\frac{1}{2}e^2\sum_{\boldsymbol{R}_n\neq 0}\frac{1}{R_n}\left[\mathrm{erfc}\left(\frac{R_n}{2\sqrt{\beta}}\right)-\mathrm{erfc}\left(\frac{R_n}{2\sqrt{\alpha}}\right)\right]\right]+\Delta E_{HF}\,, \tag{3.27}$$

where β is the Ewald parameter and $\mathrm{erfc}(x)$ is the complement of the error function $\mathrm{erf}(x)$. The ferromagnetic and antiferromagnetic two-particle exchange contributions are respectively given by

$$\Delta E_{HF}^{f} = 2N\sum_{\boldsymbol{R}_n\neq 0}e^{-R_n^2/4\alpha}\left[\frac{\hbar^2R_n^2}{32m\alpha^2}-\frac{3e^2}{2\sqrt{\pi\alpha}}-\frac{e^2}{2R_n}\mathrm{erf}\left(\frac{R_n}{2\sqrt{\alpha}}\right)\right.$$
$$+\frac{4e^2}{R_n}\mathrm{erf}\left(\frac{R_n}{4\sqrt{\alpha}}\right)+\frac{8\pi Ne^2}{\Omega}\sum_{\boldsymbol{K}_n\neq 0}\frac{e^{-\beta K_n^2}}{K_n^2}[1-e^{-\frac{1}{2}i\boldsymbol{K}_n\cdot\boldsymbol{R}_n}]$$
$$+e^2\sum_{\boldsymbol{R}_m}\frac{1}{|\boldsymbol{R}_m-\frac{1}{2}\boldsymbol{R}_n|}\left[\mathrm{erfc}\left(\frac{|\boldsymbol{R}_m-\frac{1}{2}\boldsymbol{R}_n|}{2\sqrt{\alpha}}\right)-\mathrm{erfc}\left(\frac{|\boldsymbol{R}_m-\frac{1}{2}\boldsymbol{R}_n|}{2\sqrt{\beta}}\right)\right]$$
$$\left.+e^2\sum_{\boldsymbol{R}_m}\frac{1}{R_m}\left[\mathrm{erfc}\left(\frac{R_m}{2\sqrt{\beta}}\right)-\mathrm{erfc}\left(\frac{R_m}{2\sqrt{\alpha}}\right)\right]\right] \tag{3.28}$$

and

$$\Delta E_{HF}^{a} = 2N\sum_{\boldsymbol{R}_n}e^{-R_n^2/4\alpha}\left[\frac{\hbar^2R_n^2}{32m\alpha^2}-\frac{3e^2}{2\sqrt{\pi\alpha}}-\frac{e^2}{2R_n}\mathrm{erf}\left(\frac{R_n}{2\sqrt{\alpha}}\right)+\frac{4e^2}{R_n}\mathrm{erf}\left(\frac{R_n}{4\sqrt{\alpha}}\right)\right.$$
$$+\sum_{\boldsymbol{a}=0,\boldsymbol{\delta}}\left\{\frac{4\pi Ne^2}{\Omega}\sum_{\boldsymbol{K}_n\neq 0}\frac{e^{-\beta K_n^2}}{K_n^2}e^{i\boldsymbol{K}_n\cdot\boldsymbol{a}}[1-e^{-\frac{1}{2}i\boldsymbol{K}_n\cdot\boldsymbol{R}_n}]\right.$$
$$+e^2\sum_{\boldsymbol{R}_m}\frac{1}{|\boldsymbol{R}_m+\boldsymbol{a}-\frac{1}{2}\boldsymbol{R}_n|}\left[\mathrm{erfc}\left(\frac{|\boldsymbol{R}_m+\boldsymbol{a}-\frac{1}{2}\boldsymbol{R}_n|}{2\sqrt{\alpha}}\right)-\mathrm{erfc}\left(\frac{|\boldsymbol{R}_m+\boldsymbol{a}-\frac{1}{2}\boldsymbol{R}_n|}{2\sqrt{\beta}}\right)\right]$$
$$\left.\left.+e^2\sum_{\boldsymbol{R}_m}\frac{1}{|\boldsymbol{R}_m+\boldsymbol{a}|}\left[\mathrm{erfc}\left(\frac{|\boldsymbol{R}_m+\boldsymbol{a}|}{2\sqrt{\beta}}\right)-\mathrm{erfc}\left(\frac{|\boldsymbol{R}_m+\boldsymbol{a}|}{2\sqrt{\alpha}}\right)\right]\right\}\right]\,. \tag{3.29}$$

It should be remarked here that E_{HF} does not depend on β. The sole reason for introducing this parameter is to achieve a rapid convergence of the appearing sums over

the reciprocal lattice vectors. Next we introduce the dimensionless quantities $\tilde{\alpha} = \frac{\alpha}{a_0^2}$, $\tilde{\beta} = \frac{\beta}{r_s^2 a_0^2}$, $\widetilde{\boldsymbol{R}}_n = \frac{\boldsymbol{R}_n}{r_s a_0}$, $\widetilde{\boldsymbol{K}}_n = r_s a_0 \boldsymbol{K}_n$ and $\tilde{\boldsymbol{\delta}} = \frac{\boldsymbol{\delta}}{r_s a_0}$. Then the Hartree-Fock energy can be expressed in Rydberg units reading

$$E_{HF} = 2N \left[\frac{-A}{r_s} + \frac{3}{4\tilde{\alpha}} + \frac{3\tilde{\alpha}}{r_s^3} - \frac{1}{r_s} \sum_{\widetilde{\boldsymbol{R}}_n \neq 0} \frac{1}{\tilde{R}_n} \operatorname{erfc}\left(\frac{\tilde{R}_n r_s}{2\sqrt{\tilde{\alpha}}} \right) \right] + \Delta E_{HF} \,, \tag{3.30}$$

where the Madelung constant A is given by

$$A = \frac{1}{\sqrt{\pi \tilde{\beta}}} + 3\tilde{\beta} - 3 \sum_{\widetilde{\boldsymbol{K}}_n \neq 0} \frac{1}{\tilde{K}_n^2} e^{-\tilde{\beta} \tilde{K}_n^2} - \sum_{\widetilde{\boldsymbol{R}}_n \neq 0} \frac{1}{\tilde{R}_n} \operatorname{erfc}\left(\frac{\tilde{R}_n}{2\sqrt{\tilde{\beta}}} \right) \,. \tag{3.31}$$

The relevant two-particle exchange contributions are given by

$$\begin{aligned}
\Delta E_{HF}^{f} &= 2N \sum_{\widetilde{\boldsymbol{R}}_n \neq 0} e^{-\tilde{R}_n^2 r_s^2 / 4\tilde{\alpha}} \left[\frac{\tilde{R}_n^2 r_s^2}{16\tilde{\alpha}^2} - \frac{3}{\sqrt{\pi \tilde{\alpha}}} + \frac{8}{\tilde{R}_n r_s} \operatorname{erf}\left(\frac{\tilde{R}_n r_s}{4\sqrt{\tilde{\alpha}}} \right) - \frac{1}{\tilde{R}_n r_s} \operatorname{erf}\left(\frac{\tilde{R}_n r_s}{2\sqrt{\tilde{\alpha}}} \right) \right. \\
&+ \frac{6}{r_s} \sum_{\widetilde{\boldsymbol{K}}_n \neq 0} \frac{1}{\tilde{K}_n^2} e^{-\tilde{\beta} \tilde{K}_n^2} [1 - e^{-\frac{1}{2} i \widetilde{\boldsymbol{K}}_n \cdot \widetilde{\boldsymbol{R}}_n}] \\
&+ \frac{2}{r_s} \sum_{\widetilde{\boldsymbol{R}}_m} \frac{1}{|\widetilde{\boldsymbol{R}}_m - \frac{1}{2} \widetilde{\boldsymbol{R}}_n|} \left[\operatorname{erfc}\left(\frac{|\widetilde{\boldsymbol{R}}_m - \frac{1}{2} \widetilde{\boldsymbol{R}}_n| r_s}{2\sqrt{\tilde{\alpha}}} \right) - \operatorname{erfc}\left(\frac{|\widetilde{\boldsymbol{R}}_m - \frac{1}{2} \widetilde{\boldsymbol{R}}_n|}{2\sqrt{\tilde{\beta}}} \right) \right] \\
&+ \left. \frac{2}{r_s} \sum_{\widetilde{\boldsymbol{R}}_m} \frac{1}{\tilde{R}_m} \left[\operatorname{erfc}\left(\frac{\tilde{R}_m}{2\sqrt{\tilde{\beta}}} \right) - \operatorname{erfc}\left(\frac{\tilde{R}_m r_s}{2\sqrt{\tilde{\alpha}}} \right) \right] \right]
\end{aligned} \tag{3.32}$$

and

$$\begin{aligned}
\Delta E_{HF}^{a} &= 2N \sum_{\widetilde{\boldsymbol{R}}_n \neq 0} e^{-\tilde{R}_n^2 r_s^2 / 4\tilde{\alpha}} \left[\frac{\tilde{R}_n^2 r_s^2}{16\tilde{\alpha}^2} - \frac{3}{\sqrt{\pi \tilde{\alpha}}} + \frac{8}{\tilde{R}_n r_s} \operatorname{erf}\left(\frac{\tilde{R}_n r_s}{4\sqrt{\tilde{\alpha}}} \right) - \frac{1}{\tilde{R}_n r_s} \operatorname{erf}\left(\frac{\tilde{R}_n r_s}{2\sqrt{\tilde{\alpha}}} \right) \right. \\
&+ \sum_{\tilde{\boldsymbol{a}} = 0, \tilde{\boldsymbol{\delta}}} \left\{ \frac{3}{r_s} \sum_{\widetilde{\boldsymbol{K}}_n \neq 0} \frac{1}{\tilde{K}_n^2} e^{-\tilde{\beta} \tilde{K}_n^2} e^{i \widetilde{\boldsymbol{K}}_n \cdot \tilde{\boldsymbol{a}}} [1 - e^{-\frac{1}{2} i \widetilde{\boldsymbol{K}}_n \cdot \widetilde{\boldsymbol{R}}_n}] \right. \\
&+ \frac{2}{r_s} \sum_{\widetilde{\boldsymbol{R}}_m} \frac{1}{|\widetilde{\boldsymbol{R}}_m + \tilde{\boldsymbol{a}} - \frac{1}{2} \widetilde{\boldsymbol{R}}_n|} \left[\operatorname{erfc}\left(\frac{|\widetilde{\boldsymbol{R}}_m + \tilde{\boldsymbol{a}} - \frac{1}{2} \widetilde{\boldsymbol{R}}_n| r_s}{2\sqrt{\tilde{\alpha}}} \right) - \operatorname{erfc}\left(\frac{|\widetilde{\boldsymbol{R}}_m + \tilde{\boldsymbol{a}} - \frac{1}{2} \widetilde{\boldsymbol{R}}_n|}{2\sqrt{\tilde{\beta}}} \right) \right] \\
&+ \left. \left. \frac{2}{r_s} \sum_{\widetilde{\boldsymbol{R}}_m} \frac{1}{|\widetilde{\boldsymbol{R}}_m + \tilde{\boldsymbol{a}}|} \left[\operatorname{erfc}\left(\frac{|\widetilde{\boldsymbol{R}}_m + \tilde{\boldsymbol{a}}|}{2\sqrt{\tilde{\beta}}} \right) - \operatorname{erfc}\left(\frac{|\widetilde{\boldsymbol{R}}_m + \tilde{\boldsymbol{a}}| r_s}{2\sqrt{\tilde{\alpha}}} \right) \right] \right\} \right] \,.
\end{aligned} \tag{3.33}$$

The quantities given by (3.30), (3.31), (3.32) and (3.33) must be calculated numerically. In order to check our computer program we recalculated the Madelung constants of four simple lattice structures. Our results are exactly those of Sholl [4] and are reproduced in Table I for convenience' sake. It should be mentioned here that the expression (3.31) cannot be used for the calculation of the Madelung constant of the hcp-lattice, as the attendant unit cell contains two electrons. Instead one has to start from expression (3.14) with N electrons at the lattice sites $\boldsymbol{R}_n$ of the unit cells and N electrons at the positions $\boldsymbol{R}_n + \boldsymbol{\delta}$, where $\boldsymbol{\delta}$ denotes the position of the electron inside the unit cell.

The exact value of E_{HF} up to order $S(\boldsymbol{R}_{mn})^2$ was obtained by substituting the Wigner value $\tilde{\alpha} = \frac{1}{2} r_s^{3/2}$ into (3.30), (3.32) and (3.33). As is usual we took as a measure for the stability of the lattice the energy difference between the Hartree-Fock energy E_{HF} of the Wigner lattice and the Hartree-Fock energy E_0 of the free electron gas. The energy E_0 in Rydbergs is given by [6]

$$E_0 = 2N \left(\frac{2.2099}{r_s^2} - \frac{0.9163}{r_s} \right) . \tag{3.34}$$

In fig. 1 this energy difference per electron, $\varepsilon = \dfrac{1}{2N} (E_{HF} - E_0)$, is shown for all simple ferromagnetic and antiferromagnetic lattice structures.

In order to demonstrate the influence of the two-particle exchange contributions on the width of the one-particle wave function the value of the variational parameter $\tilde{\alpha}$ was obtained numerically by minimizing E_{HF} with respect to $\tilde{\alpha}$ using an iteration procedure that starts from the Wigner value. In fig. 2 the resulting $\tilde{\alpha}$ is shown as a function of r_s for a ferromagnetic b.c.c.-lattice. Here the r_s-dependence of the Wigner $\tilde{\alpha}$ is represented as well. It appears that the other ferromagnetic and antiferromagnetic lattices give practically the same r_s-dependence of $\tilde{\alpha}$.

Summarizing, the results of the present Hartree-Fock calculations are as follows:
(1) In contrast with the classical electron system the ground state of the quantum-mechanical system is a Wigner lattice only at low densities. In the case of a b.c.c.-lattice we find that $\varepsilon = 0$ at $r_s \simeq 5$, i.e. the proposed lattice structure is not stable for higher densities.

Lattice structure	Madelung constant A
s.c.	1.76012
f.c.c.	1.79175
h.c.p.	1.79168
b.c.c.	1.79186

Table I: Madelung constants of four simple lattice structures.

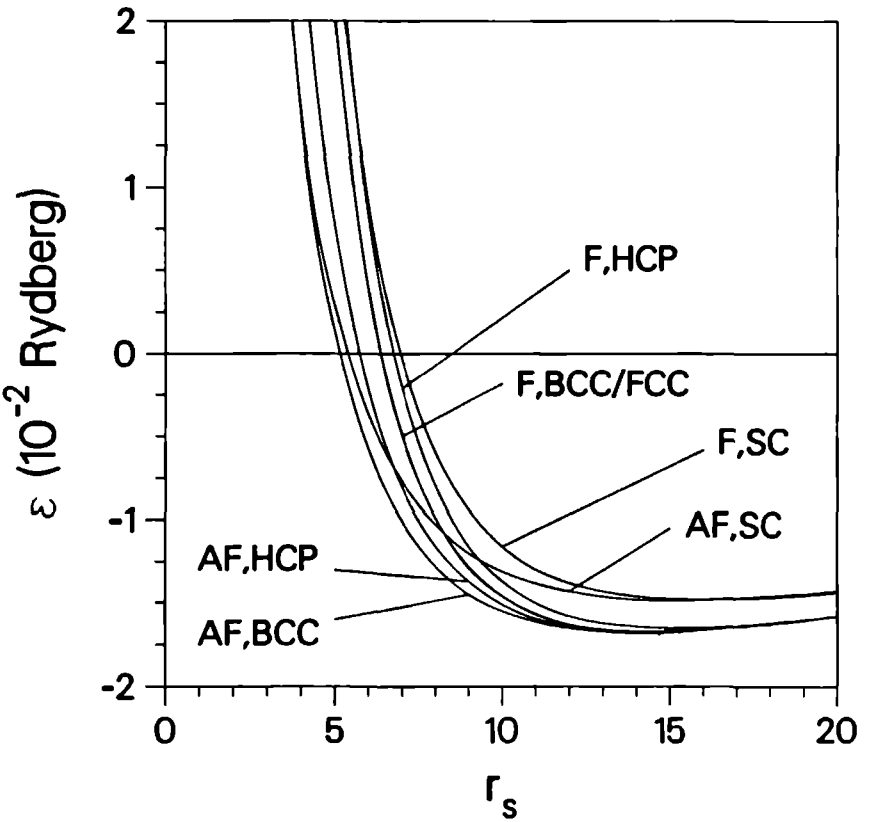

Fig. 1: Energy difference per electron, ε, between the Hartree-Fock energy of the Wigner lattice and that of the free electron gas plotted as a function of r_s for the simple ferromagnetic (F) and antiferromagnetic (AF) lattice structures.

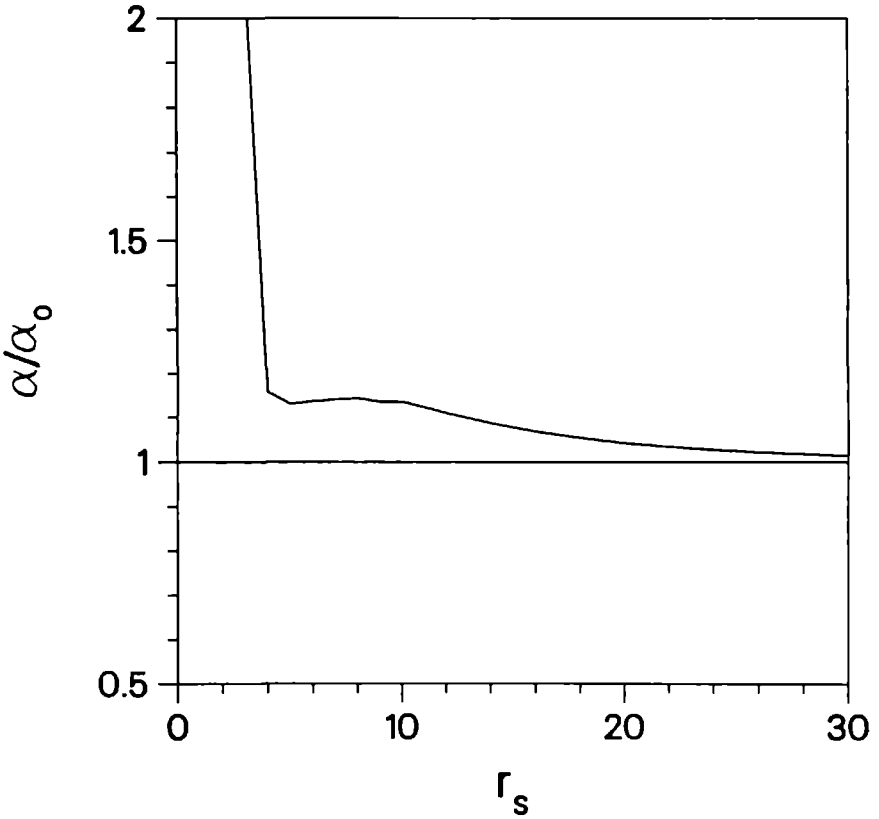

Fig. 2: Square of the width of the one-particle wave function, α, given as a function of r_s in units of the Wigner value $\alpha_0 = \frac{1}{2} r_s^{3/2} a_0^2$ for the ferromagnetic b.c.c.-lattice.

(2) The two-particle exchange contributions remove the degeneracy of the ground state with respect to all possible spin configurations of the lattice. The antiferromagnetic structure is stable compared with the ferromagnetic structure in the range $5 \lesssim r_s \lesssim 14$, the ferromagnetic structure has the lowest energy at lower densities, $r_s > 14$. In that region, however, the energy difference between both structures is extremely small. Consequently a small inaccuracy in the calculation of the two-particle exchange contributions can produce a large error in the critical value of r_s where both lattices have equal energy. As is shown in Appendix IV this accounts for the discrepancy between our critical value $r_s = 14$ and Carr's result $r_s = 270$ [5].

(3) The exchange influences the width of the localized one-electron wave functions. It appears that the width increases with respect to the Wigner value, i.e. the wave packets become less localized.

4. Correlation in the Wigner lattice

The effect of correlation on the HF ground state energy has been discussed by Carr [5]. He replaced the original Wigner lattice of uncoupled oscillators by a lattice of coupled oscillators. The semi-classical nature of his approach, however, raises some epistemological questions. In order to discuss these questions properly we first summarize Carr's approach.

By analogy with Born's lattice theory [7] Carr expanded the electron-electron interaction around the equilibrium positions $\boldsymbol{R}_i$ of the electrons. These positions are thought to form a lattice. The expansion in terms of the displacements $\boldsymbol{r}_i - \boldsymbol{R}_i$ gives rise to the following Hamiltonian for the electron system:

$$H = E_{Cl} + \sum_i \frac{\boldsymbol{p}_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} (\boldsymbol{r}_i - \boldsymbol{R}_i) \boldsymbol{M}(\boldsymbol{R}_{ij}) (\boldsymbol{r}_j - \boldsymbol{R}_j) + \ldots , \tag{4.1}$$

where E_{Cl} denotes the Madelung energy of the classical electron lattice. The elements $M(\boldsymbol{R}_{ij})_{\mu\nu}$, with $\mu, \nu = x, y, z$, of the second rank tensor $\boldsymbol{M}(\boldsymbol{R}_{ij})$ are given by

$$\begin{aligned} M(\boldsymbol{R}_{ij})_{\mu\nu} &= \frac{\partial^2}{\partial R_i^\mu \partial R_j^\nu} \left(\frac{e^2}{|\boldsymbol{R}_i - \boldsymbol{R}_j|} \right) \quad , \quad i \neq j \, , \\ M(0)_{\mu\nu} &= \frac{8\pi N e^2}{3\Omega} \delta_{\mu\nu} \, . \end{aligned} \tag{4.2}$$

Neglecting the anharmonic terms in the expansion (4.1) the remaining problem was solved in the familiar way by introducing the normal coordinates

$$\begin{aligned} q_{\boldsymbol{k}\lambda} &= \frac{1}{\sqrt{2N}} \sum_i e^{i\boldsymbol{k} \cdot \boldsymbol{R}_i} \boldsymbol{\varepsilon}_{\boldsymbol{k}\lambda} \cdot (\boldsymbol{r}_i - \boldsymbol{R}_i) \, , \\ p_{\boldsymbol{k}\lambda} &= \frac{1}{\sqrt{2N}} \sum_i e^{i\boldsymbol{k} \cdot \boldsymbol{R}_i} \boldsymbol{\varepsilon}_{\boldsymbol{k}\lambda} \cdot \boldsymbol{p}_i \, , \end{aligned} \tag{4.3}$$

with $2N$ denoting the number of electrons and $\boldsymbol{k}$ and λ being the wave vector and polarization index ($\lambda = 1, 2, 3$) of the vibrational eigenmodes, respectively. The polarization vectors $\boldsymbol{\varepsilon}_{\boldsymbol{k}\lambda}$ are determined by the eigenvalue equation

$$\sum_i e^{i\boldsymbol{k} \cdot \boldsymbol{R}_{ij}} \boldsymbol{M}(\boldsymbol{R}_{ij}) \boldsymbol{\varepsilon}_{\boldsymbol{k}\lambda} = m\omega_{\boldsymbol{k}\lambda}^2 \boldsymbol{\varepsilon}_{\boldsymbol{k}\lambda} \, , \tag{4.4}$$

where $\omega_{\boldsymbol{k}\lambda}$ is the frequency of an eigenmode. Next the quantum nature of the system was taken into account by requiring $[q_{\boldsymbol{k}\lambda}, p_{\boldsymbol{k}'\lambda'}] = i\hbar \, \delta_{\boldsymbol{k}\boldsymbol{k}'} \delta_{\lambda\lambda'}$. Introducing the boson

operators

$$a^+_{\boldsymbol{k}\lambda} = [2\hbar\, m\omega_{\boldsymbol{k}\lambda}]^{-1/2}[m\omega_{\boldsymbol{k}\lambda}\, q_{-\boldsymbol{k}\lambda} - ip_{\boldsymbol{k}\lambda}]$$
$$a_{\boldsymbol{k}\lambda} = [2\hbar\, m\omega_{\boldsymbol{k}\lambda}]^{-1/2}[m\omega_{\boldsymbol{k}\lambda}\, q_{\boldsymbol{k}\lambda} + ip_{-\boldsymbol{k}\lambda}] \tag{4.5}$$

the following Hamiltonian resulted for the low density electron system:

$$H_C = E_{CI} + \sum_{\boldsymbol{k}\lambda} \hbar\omega_{\boldsymbol{k}\lambda} \left[\frac{1}{2} + a^+_{\boldsymbol{k}\lambda} a_{\boldsymbol{k}\lambda}\right] . \tag{4.6}$$

After calculating the eigenfrequencies from (4.4) and performing the sum over $\boldsymbol{k}$ and λ by using a numerical integration procedure Carr arrived at a ground state energy in Rydberg units given by

$$E_C^{(0)} = 2N\left(\frac{-A}{r_s} + \frac{2.66}{r_s^{3/2}}\right) = E_H^{(0)} - 2N\,\frac{0.34}{r_s^{3/2}} , \tag{4.7}$$

where $E_H^{(0)}$ is the Wigner ground state energy (3.21).

The ground state $|\varphi_{\text{harm}}\rangle$ that belongs to the energy (4.7), is found by the requirement

$$a_{\boldsymbol{k}\lambda}|\varphi_{\text{harm}}\rangle = 0 , \tag{4.8}$$

for all $\boldsymbol{k}$ and λ. In coordinate-language this ground state is represented by the wave function

$$\begin{aligned}\varphi_{\text{harm}}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_{2N}) &= \prod_{\boldsymbol{k},\lambda}\left(\frac{m\omega_{\boldsymbol{k}\lambda}}{\pi\boldsymbol{k}}\right)^{1/4} \exp\left[-\frac{m\omega_{\boldsymbol{k}\lambda}}{2\hbar}\, q_{\boldsymbol{k}\lambda}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_{2N}) q_{-\boldsymbol{k}\lambda}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_{2N})\right] \\ &= \exp\left[-\sum_{i\neq j} u_{ij}(\boldsymbol{r}_i,\boldsymbol{r}_j)\right] \prod_{i=1}^{2N} f(\boldsymbol{r}_i - \boldsymbol{R}_i) ,\end{aligned} \tag{4.9}$$

where the functions f and u_{ij} are given by, respectively,

$$\begin{aligned} f(\boldsymbol{r}_i - \boldsymbol{R}_i) &= \left[\prod_{\boldsymbol{k}\lambda}\left(\frac{m\omega_{\boldsymbol{k}\lambda}}{2\hbar}\right)\right]^{1/2N} \\ &\times \exp\left[\frac{-1}{2N}\sum_{\boldsymbol{k}\lambda}\left(\frac{m\omega_{\boldsymbol{k}\lambda}}{2\hbar}\right)[(\boldsymbol{r}_i - \boldsymbol{R}_i)\cdot\boldsymbol{\varepsilon}_{\boldsymbol{k}\lambda}]\,[\boldsymbol{\varepsilon}_{-\boldsymbol{k}\lambda}\cdot(\boldsymbol{r}_i - \boldsymbol{R}_i)]\right] \\ u_{ij}(\boldsymbol{r}_i,\boldsymbol{r}_j) &= \frac{1}{2N}\sum_{\boldsymbol{k}\lambda}\left(\frac{m\omega_{\boldsymbol{k}\lambda}}{2\hbar}\right) e^{i\boldsymbol{k}\cdot\boldsymbol{R}_{ij}}[(\boldsymbol{r}_i - \boldsymbol{R}_i)\cdot\boldsymbol{\varepsilon}_{\boldsymbol{k}\lambda}]\,[\boldsymbol{\varepsilon}_{-\boldsymbol{k}\lambda}\cdot(\boldsymbol{r}_j - \boldsymbol{R}_j)] . \end{aligned} \tag{4.10}$$

Clearly $\varphi_{\text{harm}}(\mathbf{r}_1, \ldots, \mathbf{r}_{2N})$ is not antisymmetric in the coordinates of the electrons, i.e. this wave function cannot describe the ground state of the low density electron system as the effect of exchange is excluded. In order to estimate a posteriori the magnitude of this neglected contribution to the ground state energy Carr calculated, starting from a basis set of Slater determinants of harmonic oscillator wave functions, the matrix elements of the total Hamiltonian. It appeared that the exchange terms fell off like $\exp(-Cr_s^{1/2})$, where C is some constant. Therefore he concluded that the expansion of the Hamiltonian (4.1) leads to exact results provided that all these exponential terms can be neglected. Then the expression (4.7) for the ground state energy of the low density electron system is exact up to order $r_s^{-3/2}$.

In our opinion Carr's result (4.7) for the ground state energy is correct, but his approach raises the following epistemological questions.

(1) The Hamiltonian, which is obtained after breaking off the expansion (4.1), is no longer invariant under the permutation of the coordinates of the electrons. This means that the electrons are conceived as distinguishable particles, i.e. Carr's approach violates an important quantummechanical principle. The resulting system of distinguishable electrons vibrating around their equilibrium positions is then considered as a quantum system and dealt with accordingly. The question is now whether it is possible to derive Carr's result in a fully quantummechanical way, i.e. without violating the permutation symmetry.

(2) Carr describes the electrons in terms of boson operators known as phonons. The introduction of the phonon concept, however, is only a mathematical convenience. Consequently a well-defined relation between the boson operators (4.5) and the original fermion operators describing the creation and annihilation of electrons must exist. What is the form of that relation?

(3) The semiclassical approach of Carr does not lead to an antisymmetric ground state wave function with the energy as given in (4.7). According to Carr that wave function can in principle be calculated a posteriori by diagonalizing the Hamiltonian matrix that is obtained from the complete set of Slater determinants of harmonic oscillator wave func-

tions, which are the solutions of (4.6). However Carr does not give an algorithm needed to actually perform this calculation. It seems plausible that the antisymmetric wave function based upon (4.9), i.e.

$$|\varphi^{A}_{\rm harm}\rangle = \int d^3r_1 \ldots d^3r_{2N}\, \varphi_{\rm harm}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_{2N})\, \psi^{+}_{\tau_1}(\boldsymbol{r}_1) \ldots \psi^{+}_{\tau_{2N}}(\boldsymbol{r}_{2N})|\rangle \ , \qquad (4.11)$$

might possibly lead to the required energy (4.7), provided that all exponential terms appearing in the energy expression are neglected. It should be remarked, however, that such a suggestion is still unfounded. Obviously a fully quantummechanical approach leads in principle directly to an antisymmetric ground state wave function. The question is then how to obtain that wave function.

A possible way to answer the posed questions is to use the variational method starting with an Ansatz of the form (4.11) for the wave function. That would be a logical continuation of the approach discussed in section 3. Unfortunately, such an Ansatz is too complicated in the present case. In fact any variational calculation, that is based upon an Ansatz for a many-electron wave function unlike the Hartree-Fock type, is extremely difficult. Therefore another method must be looked for, that should preferably reproduce the original Wigner result as well. Here we introduce a fully quantummechanical approach, which is partly based on work by Brenig [8], Fredkin and Werthamer [9] and Pietrass [10].

The starting point of the present approach is to represent the eigenstates of the low density electron system as linear combinations of Slater determinants of one-electron states. Such a decomposition is always possible provided that these one-electron states form a complete set. In view of the results already obtained in section 3 the set of eigenstates of the harmonic oscillator is an obvious choice. The important consequence of this choice is that the decompositions of the system's ground state and low lying excited states involve only a limited number of important terms, namely those terms that contain the ground state and the low lying states of the harmonic oscillator. In terms of the Cartesian coordinates x, y, z the harmonic oscillator eigenfunctions are given by

$$f_{\boldsymbol{\jmath}}(\boldsymbol{r}) = \prod_{\hat{\boldsymbol{\xi}}} [\sqrt{2\alpha\pi}\, 2^{\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}}\, (\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}})!]^{-1/2} \exp\left[\frac{-(\boldsymbol{r}\cdot\hat{\boldsymbol{\xi}})^2}{4\alpha}\right] H_{\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}}\left(\frac{\boldsymbol{r}\cdot\hat{\boldsymbol{\xi}}}{\sqrt{2\alpha}}\right) \ , \qquad (4.12)$$

where $\hat{\boldsymbol{\xi}}$ runs over the basis vectors, $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$ and $\hat{\boldsymbol{z}}$ of a given Cartesian coordinate system, $\boldsymbol{\jmath} = (j_x, j_y, j_z)$, $\boldsymbol{\jmath} \cdot \hat{\boldsymbol{\xi}} = 0, 1, 2, \ldots$, and $H_{\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}}$ is the Hermite polynomial of order $\boldsymbol{\jmath} \cdot \hat{\boldsymbol{\xi}}$. The width $\alpha^{1/2}$ of the functions $f_{\boldsymbol{\jmath}}$ is still arbitrary. In terms of the given one-electron functions the eigenstates $|\psi_n\rangle$ of a low density electron system consisting of $2N$ electrons can be expressed as (cf. (3.7))

$$|\psi_n\rangle = \sum_{\substack{\boldsymbol{\jmath}_1, \boldsymbol{\jmath}_2, \ldots, \boldsymbol{\jmath}_{2N} \\ \boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \ldots, \boldsymbol{\sigma}_{2N}}} A^{\sigma_1 \ldots \sigma_{2N}}_{\boldsymbol{\jmath}_1 \ldots \boldsymbol{\jmath}_{2N}}(n)\, d^{+}_{\boldsymbol{\jmath}_1\sigma_1}(\boldsymbol{R}_1) \ldots d^{+}_{\boldsymbol{\jmath}_{2N}\sigma_{2N}}(\boldsymbol{R}_{2N})|\rangle\,, \tag{4.13}$$

where the operator $d^{+}_{\boldsymbol{\jmath}_i\sigma_i}(\boldsymbol{R}_i)$ describes the creation of an electron with spin σ_i in the harmonic oscillator eigenfunction $f_{\boldsymbol{\jmath}_i}$ localized around lattice site $\boldsymbol{R}_i$:

$$\begin{aligned} d^{+}_{\boldsymbol{\jmath}_i\sigma_i}(\boldsymbol{R}_i) &= \int d^3r\, \psi^{+}_{\sigma_i}(\boldsymbol{r})\, f_{\boldsymbol{\jmath}_i}(\boldsymbol{r} - \boldsymbol{R}_i) \\ &= \left[\frac{(2\pi)^3}{\Omega}\right]^{1/2} \sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_i}\, \hat{f}_{\boldsymbol{\jmath}_i}(\boldsymbol{k}) c^{+}_{\boldsymbol{k}\sigma_i}\,, \end{aligned} \tag{4.14}$$

with $\hat{f}_{\boldsymbol{\jmath}_i}$ being the Fourier transform of $f_{\boldsymbol{\jmath}_i}$, i.e.

$$\begin{aligned} \hat{f}_{\boldsymbol{\jmath}}(\boldsymbol{k}) &= \frac{1}{(2\pi)^{3/2}} \int d^3r\, f_{\boldsymbol{\jmath}}(\boldsymbol{r})\, e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} \\ &= \prod_{\hat{\boldsymbol{\xi}}} (-i)^{\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}} \left[\sqrt{\frac{\pi}{2\alpha}}\, 2^{\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}}\, (\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}})!\right]^{-\frac{1}{2}} \exp[-\alpha(\boldsymbol{k}\cdot\hat{\boldsymbol{\xi}})^2] H_{\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}}(\boldsymbol{k}\cdot\hat{\boldsymbol{\xi}}\sqrt{2\alpha})\,. \end{aligned} \tag{4.15}$$

The proposed decomposition (4.13) has the great merit of showing that the exchange contribution to the energy of the ground state and the low lying excited states of the low density electron system can be neglected in a first approximation. That can be concluded directly from the following two considerations. First of all the coefficients $A^{\sigma_1 \ldots \sigma_{2N}}_{\boldsymbol{\jmath}_1 \ldots \boldsymbol{\jmath}_{2N}}(n)$ tend rapidly to zero with increasing $|\boldsymbol{\jmath}_1|, \ldots, |\boldsymbol{\jmath}_{2N}|$ for the ground state and the low lying excited states. Secondly the overlap between one-electron functions, that are centered around different lattice positions is quite small for small $|\boldsymbol{\jmath}_i|$. This follows immediately

from the expression for the overlap

$$S_{\boldsymbol{\jmath}_1,\boldsymbol{\jmath}_2}(\boldsymbol{R}_{12}) = \int d^3r f^*_{\boldsymbol{\jmath}_1}(\boldsymbol{r}-\boldsymbol{R}_1) f_{\boldsymbol{\jmath}_2}(\boldsymbol{r}-\boldsymbol{R}_2)$$

$$= \exp\left[\frac{-R_{12}^2}{8\alpha}\right] \prod_{\hat{\boldsymbol{\xi}}} \left[\frac{2\jmath_>\cdot\hat{\boldsymbol{\xi}}(\jmath_<\cdot\hat{\boldsymbol{\xi}})!}{2\jmath_<\cdot\hat{\boldsymbol{\xi}}(\jmath_>\cdot\hat{\boldsymbol{\xi}})!}\right]^{1/2} \left(\frac{\boldsymbol{R}_{12}\cdot\hat{\boldsymbol{\xi}}}{2\sqrt{2\alpha}}\right)^{(\jmath_>-\jmath_<)\cdot\hat{\boldsymbol{\xi}}} L^{(\jmath_>-\jmath_<)\cdot\hat{\boldsymbol{\xi}}}_{\jmath_<\cdot\hat{\boldsymbol{\xi}}}\left(\frac{(\boldsymbol{R}_{12}\cdot\hat{\boldsymbol{\xi}})^2}{4\alpha}\right) , \tag{4.16}$$

where $L^{(\jmath_>-\jmath_<)\cdot\hat{\boldsymbol{\xi}}}_{\jmath_<\cdot\hat{\boldsymbol{\xi}}}$ denotes a Laguerre polynomial with $\jmath_>\cdot\hat{\boldsymbol{\xi}}$ and $\jmath_<\cdot\hat{\boldsymbol{\xi}}$ being the larger and the smaller of the two numbers $\{\boldsymbol{\jmath}_1\cdot\hat{\boldsymbol{\xi}}, \boldsymbol{\jmath}_2\cdot\hat{\boldsymbol{\xi}}\}$, respectively. Clearly $S_{\boldsymbol{\jmath}_1\boldsymbol{\jmath}_2}(\boldsymbol{R}_{12})$ is very small at low densities, provided that both the width $\alpha^{1/2}$ of the one-electron functions is small compared with the nearest neighbour distance and the exponential factor dominates (4.16), i.e. $|\boldsymbol{\jmath}_1|$ and $|\boldsymbol{\jmath}_2|$ should not become too large.

In the following we pay attention to the properties of the low density electron system at low temperatures, i.e. we are only interested in the ground state and the low-lying excited states. Our conclusion that the influence of the exchange energy on the low temperature properties can be neglected in a first approximation can be expressed mathematically by putting

$$\{d^+_{\boldsymbol{\jmath}_1\sigma_1}(\boldsymbol{R}_1), d_{\boldsymbol{\jmath}_2\sigma_2}(\boldsymbol{R}_2)\} = S_{\boldsymbol{\jmath}_1\boldsymbol{\jmath}_2}(\boldsymbol{R}_{12})\delta_{\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2} = \delta_{\boldsymbol{\jmath}_1\boldsymbol{\jmath}_2}\delta_{\boldsymbol{R}_1\boldsymbol{R}_2}\delta_{\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2} . \tag{4.17}$$

The crucial step in our approach is to use the decomposition (4.13) in order to find an effective Hamiltonian with the property

$$H_{\text{eff}}|\psi_n\rangle = E_n|\psi_n\rangle , \tag{4.18}$$

where E_n is the approximate energy of the low lying eigenstate $|\psi_n\rangle$ as given in (4.13), i.e. the exchange contribution to the energy spectrum is neglected. The reason for the formulation of an effective Hamiltonian is to analyze the dynamics of the system without taking into account the effect of exchange. In order to construct H_{eff} we first rewrite H, as given in (3.1), in terms of the fermion operators (4.14). For that purpose we use the following relation between plane wave functions and oscillator eigenfunctions:

$$\exp[i\boldsymbol{k}\cdot\boldsymbol{r}] = (2\pi)^{3/2}\sum_{\boldsymbol{\jmath}} e^{i\boldsymbol{k}\cdot\boldsymbol{a}} f^*_{\boldsymbol{\jmath}}(\boldsymbol{r}-\boldsymbol{a})\hat{f}_{\boldsymbol{\jmath}}(\boldsymbol{k}) , \tag{4.19}$$

where $\boldsymbol{a}$ denotes the position around which the function $f_{\boldsymbol{\jmath}}$ is localized. This relation follows directly from the completeness of the set of harmonic oscillator eigenfunctions, i.e.

$$\sum_{\boldsymbol{\jmath}} f^*_{\boldsymbol{\jmath}}(\boldsymbol{r})f_{\boldsymbol{\jmath}}(\boldsymbol{r}') = \delta^3(\boldsymbol{r}-\boldsymbol{r}') \; . \tag{4.20}$$

The required relation between the different sets of fermion operators then reads

$$c^+_{\boldsymbol{k}\sigma} = \frac{1}{\sqrt{\Omega}} \int d^3r \, \psi^+_\sigma(\boldsymbol{r}) \, e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = \left[\frac{(2\pi)^3}{\Omega}\right]^{1/2} \sum_{\boldsymbol{\jmath}} \hat{f}_{\boldsymbol{\jmath}}(\boldsymbol{k}) \, e^{i\boldsymbol{k}\cdot\boldsymbol{a}} \, d^+_{\boldsymbol{\jmath}\sigma}(\boldsymbol{a}) \; . \tag{4.21}$$

N.B. The vector $\boldsymbol{a}$ can be arbitrarily chosen. This freedom is essential for obtaining the effective Hamiltonian.

Substitution of (4.21) into (3.1) while taking into account the arbitrariness of $\boldsymbol{a}$ gives rise to the following possible representation of H:

$$\begin{aligned} H \;\; = \;\; & \sum_{\boldsymbol{\jmath}_1\boldsymbol{\jmath}_2,\sigma} T^{\boldsymbol{a}_1\boldsymbol{a}_2}_{\boldsymbol{\jmath}_1\boldsymbol{\jmath}_2} \, d^+_{\boldsymbol{\jmath}_1\sigma}(\boldsymbol{a}_1) d_{\boldsymbol{\jmath}_2\sigma}(\boldsymbol{a}_2) \\ & + \; \frac{1}{2} \sum_{\substack{\boldsymbol{\jmath}_3\boldsymbol{\jmath}_4\boldsymbol{\jmath}_5\boldsymbol{\jmath}_6 \\ \sigma,\sigma'}} V^{\boldsymbol{a}_3\boldsymbol{a}_4\boldsymbol{a}_5\boldsymbol{a}_6}_{\boldsymbol{\jmath}_3\boldsymbol{\jmath}_4\boldsymbol{\jmath}_5\boldsymbol{\jmath}_6} \, d^+_{\boldsymbol{\jmath}_3\sigma}(\boldsymbol{a}_3) d^+_{\boldsymbol{\jmath}_4\sigma'}(\boldsymbol{a}_4) d_{\boldsymbol{\jmath}_5\sigma'}(\boldsymbol{a}_5) d_{\boldsymbol{\jmath}_6\sigma}(\boldsymbol{a}_6) \; , \end{aligned} \tag{4.22}$$

with

$$T^{\boldsymbol{a}_1\boldsymbol{a}_2}_{\boldsymbol{\jmath}_1\boldsymbol{\jmath}_2} = \int d^3k \, \frac{\hbar^2k^2}{2m} \, e^{i\boldsymbol{k}\cdot(\boldsymbol{a}_1-\boldsymbol{a}_2)} \, \hat{f}^*_{\boldsymbol{\jmath}_2}(\boldsymbol{k}) f_{\boldsymbol{\jmath}_1}(\boldsymbol{k}) \; , \tag{4.23}$$

$$V^{\boldsymbol{a}_3\boldsymbol{a}_4\boldsymbol{a}_5\boldsymbol{a}_6}_{\boldsymbol{\jmath}_3\boldsymbol{\jmath}_4\boldsymbol{\jmath}_5\boldsymbol{\jmath}_6} = {\sum_{\boldsymbol{q}}}' \frac{4\pi e^2}{\Omega q^2} \, e^{i\boldsymbol{q}\cdot(\boldsymbol{a}_6-\boldsymbol{a}_5)} \Big[$$

$$\int d^3k d^3k' \, \hat{f}_{\boldsymbol{\jmath}_3}(\boldsymbol{k}) \hat{f}_{\boldsymbol{\jmath}_4}(\boldsymbol{k}') \hat{f}^*_{\boldsymbol{\jmath}_5}(\boldsymbol{k}'+\boldsymbol{q}) \hat{f}^*_{\boldsymbol{\jmath}_6}(\boldsymbol{k}-\boldsymbol{q}) \, e^{i\boldsymbol{k}\cdot(\boldsymbol{a}_3-\boldsymbol{a}_6)} \, e^{i\boldsymbol{k}'(\boldsymbol{a}_4-\boldsymbol{a}_5)} \Big] . \tag{4.24}$$

Clearly different sets of vectors $\boldsymbol{a}_\ell$, $\ell = 1,2,\ldots,6$, correspond with different representations of the same Hamiltonian H, i.e. the eigenfunctions and eigenvalues of H do not depend on the choice of $\boldsymbol{a}_\ell$ or, to put it differently, the translational symmetry of H is not

broken. The reason for introducing the representation (4.22) becomes clear when considering $H|\psi_n\rangle$. Using the decomposition (4.13) and the procedure as given in Appendix I (cf. I.4) we get

$$H|\psi_n\rangle = \sum_{\substack{\boldsymbol{\jmath}_1,\ldots,\boldsymbol{\jmath}_{2N} \\ \sigma_1,\ldots,\sigma_{2N}}} A^{\sigma_1,\ldots,\sigma_{2N}}_{\boldsymbol{\jmath}_1,\ldots,\boldsymbol{\jmath}_{2N}}(n) \left\{ \sum_{\imath=1}^{2N} (-1)^{2N-\imath} \left[\prod_{m\neq\imath} d^+_{\boldsymbol{\jmath}_m\sigma_m}(\boldsymbol{R}_m) \right] \left[H, d^+_{\boldsymbol{\jmath}_\imath\sigma_\imath}(\boldsymbol{R}_\imath)\right] |\rangle \right.$$

$$\left. + \sum_{\imath=1}^{2N} \sum_{\jmath=\imath+1}^{2N} (-1)^{-\imath+\jmath+1} \left[\prod_{m\neq\imath,\jmath} d^+_{\boldsymbol{\jmath}_m\sigma_m}(\boldsymbol{R}_m) \right] \left\{ \left[H, d^+_{\boldsymbol{\jmath}_\imath\sigma_\imath}(\boldsymbol{R}_\imath)\right], d^+_{\boldsymbol{\jmath}_\jmath\sigma_\jmath}(\boldsymbol{R}_\jmath) \right\} |\rangle \right\}. \tag{4.25}$$

The appearing commutators are calculated by using suitably chosen representations of H, i.e. we choose a different set $\boldsymbol{a}_\ell$, $\ell = 1,2,\ldots,6$, for each commutator. Calling this set $\boldsymbol{a}^\imath_1, \boldsymbol{a}^\imath_2, \boldsymbol{a}^\imath_3, \boldsymbol{a}^\jmath_4, \boldsymbol{a}^\jmath_5, \boldsymbol{a}^\imath_6$, we arrive at

$$[H, d^+_{\boldsymbol{\jmath}_\imath\sigma_\imath}(\boldsymbol{R}_\imath)]|\rangle = \sum_{\imath_1\imath_2} T^{\boldsymbol{a}^\imath_1\boldsymbol{a}^\imath_2}_{\imath_1\imath_2} S_{\boldsymbol{\jmath}_\imath\imath_2}(\boldsymbol{R}_\imath - \boldsymbol{a}^\imath_2) d^+_{\imath_1\sigma_\imath}(\boldsymbol{a}^\imath_1)|\rangle$$

$$\{[H, d^+_{\boldsymbol{\jmath}_\imath\sigma_\imath}(\boldsymbol{R}_\imath)], d^+_{\boldsymbol{\jmath}_\jmath\sigma_\jmath}(\boldsymbol{R}_\jmath)\}|\rangle = \sum_{\imath_3\imath_4\imath_5\imath_6} V^{\boldsymbol{a}^\imath_3\boldsymbol{a}^\jmath_4\boldsymbol{a}^\jmath_5\boldsymbol{a}^\imath_6}_{\imath_3\imath_4\imath_5\imath_6}$$

$$\times S_{\boldsymbol{\jmath}_\imath\imath_6}(\boldsymbol{R}_\imath - \boldsymbol{a}^\imath_6)\, S_{\boldsymbol{\jmath}_\jmath\imath_5}(\boldsymbol{R}_\jmath - \boldsymbol{a}^\jmath_5) d^+_{\imath_3\sigma_\imath}(\boldsymbol{a}^\imath_3) d^+_{\imath_4\sigma_\jmath}(\boldsymbol{a}^\jmath_4)|\rangle\ . \tag{4.26}$$

A further simplification of (4.26) is obtained by the special choice $\boldsymbol{a}^\imath_1 = \boldsymbol{a}^\imath_2 = \boldsymbol{a}^\imath_3 = \boldsymbol{a}^\imath_6 = \boldsymbol{R}_\imath$ and $\boldsymbol{a}^\jmath_4 = \boldsymbol{a}^\jmath_5 = \boldsymbol{R}_\jmath$. Then the overlap integrals in (4.26) are equal to one. Now the effective Hamiltonian can be formulated. For the resulting exact expression for $H|\psi_n\rangle$, given by (4.25) and (4.26), can also be obtained by replacing H by the following effective Hamiltonian H_{eff}, provided that the overlap terms are neglected:

$$H_{\text{eff}} = \sum_{\imath,\boldsymbol{\jmath}_1,\boldsymbol{\jmath}_2,\sigma} T_{\boldsymbol{\jmath}_1\boldsymbol{\jmath}_2}\, d^+_{\boldsymbol{\jmath}_1\sigma}(\boldsymbol{R}_\imath) d_{\boldsymbol{\jmath}_2\sigma}(\boldsymbol{R}_\imath)$$

$$+ \frac{1}{2} \sum_{\imath\neq\jmath} \sum_{\boldsymbol{\jmath}_3\boldsymbol{\jmath}_4\boldsymbol{\jmath}_5\boldsymbol{\jmath}_6,\sigma\sigma'} V^{\imath\jmath}_{\boldsymbol{\jmath}_3\boldsymbol{\jmath}_4\boldsymbol{\jmath}_5\boldsymbol{\jmath}_6} d^+_{\boldsymbol{\jmath}_3\sigma}(\boldsymbol{R}_\imath) d^+_{\boldsymbol{\jmath}_4\sigma'}(\boldsymbol{R}_\jmath) d^+_{\boldsymbol{\jmath}_5\sigma'}(\boldsymbol{R}_\jmath) d^+_{\boldsymbol{\jmath}_6\sigma}(\boldsymbol{R}_\imath), \tag{4.27}$$

where

$$T_{\mathcal{J}_1\mathcal{J}_2} = \int d^3k \frac{\hbar^2 k^2}{2m} \hat{f}_{\mathcal{J}_2}(\boldsymbol{k}) \hat{f}_{\mathcal{J}_1}(\boldsymbol{k})$$

$$= \sum_{\hat{\boldsymbol{\xi}} \in \{\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}, \hat{\boldsymbol{z}}\}} \frac{\hbar^2}{4m\alpha} \left[\delta_{\mathcal{J}_1\mathcal{J}_2} (\mathcal{J}_1 \cdot \hat{\boldsymbol{\xi}} + \frac{1}{2}) - \frac{1}{2} \delta_{\mathcal{J}_1, \mathcal{J}_2 + 2\hat{\boldsymbol{\xi}}} \sqrt{(\mathcal{J}_2 \cdot \hat{\boldsymbol{\xi}} + 1)(\mathcal{J}_2 \cdot \hat{\boldsymbol{\xi}} + 2)} \right.$$

$$\left. - \frac{1}{2} \delta_{\mathcal{J}_2, \mathcal{J}_1 + 2\hat{\boldsymbol{\xi}}} \sqrt{(\mathcal{J}_1 \cdot \hat{\boldsymbol{\xi}} + 1)(\mathcal{J}_1 \cdot \hat{\boldsymbol{\xi}} + 2)} \right] \tag{4.28}$$

and

$$V^{ij}_{\mathcal{J}_3\mathcal{J}_4\mathcal{J}_5\mathcal{J}_6} = \sum_{\boldsymbol{q}}{}' \frac{4\pi e^2}{\Omega q^2} e^{i\boldsymbol{q} \cdot \boldsymbol{R}_{ij}} \int d^3k d^3k' \, \hat{f}_{\mathcal{J}_3}(\boldsymbol{k}) \hat{f}_{\mathcal{J}_4}(\boldsymbol{k}') \hat{f}^*_{\mathcal{J}_5}(\boldsymbol{k}' + \boldsymbol{q}) \hat{f}^*_{\mathcal{J}_6}(\boldsymbol{k} - \boldsymbol{q}) \tag{4.29}$$

with

$$\int d^3k \hat{f}_{\boldsymbol{\ell}_1}(\boldsymbol{k}) \hat{f}^*_{\boldsymbol{\ell}_2}(\boldsymbol{k} \pm \boldsymbol{q}) =$$

$$e^{-\frac{1}{2}\alpha q^2} \prod_{\hat{\boldsymbol{\xi}}} \left[\frac{2^{\boldsymbol{\ell}_> \cdot \hat{\boldsymbol{\xi}}} (\boldsymbol{\ell}_< \cdot \hat{\boldsymbol{\xi}})}{2^{\boldsymbol{\ell}_< \cdot \hat{\boldsymbol{\xi}}} (\boldsymbol{\ell}_> \cdot \hat{\boldsymbol{\xi}})} \right]^{1/2} (\pm i \frac{1}{2} \sqrt{2\alpha} \, \boldsymbol{q} \cdot \hat{\boldsymbol{\xi}})^{(\boldsymbol{\ell}_> - \boldsymbol{\ell}_<) \cdot \hat{\boldsymbol{\xi}}} \, L^{(\boldsymbol{\ell}_> - \boldsymbol{\ell}_<) \cdot \hat{\boldsymbol{\xi}}}_{\boldsymbol{\ell}_< \cdot \hat{\boldsymbol{\xi}}} (\alpha (\boldsymbol{q} \cdot \hat{\boldsymbol{\xi}})^2). \tag{4.30}$$

The Hamiltonian (4.27) does not take into account the effect of exchange on the dynamics of the electrons. Note that the original translation symmetry is broken in H_{eff}.

Next H_{eff} is expressed in terms of the following electron-hole operators.

$$D^i_{\mathcal{J}_1\mathcal{J}_2} = \sum_{\sigma} d^+_{\mathcal{J}_1\sigma}(\boldsymbol{R}_i) d_{\mathcal{J}_2\sigma}(\boldsymbol{R}_i) \, . \tag{4.31}$$

Substituting (4.31) into (4.27) we obtain

$$H_{\text{eff}} = \sum_i \sum_{\mathcal{J}_1\mathcal{J}_2} T_{\mathcal{J}_1\mathcal{J}_2} D^i_{\mathcal{J}_1\mathcal{J}_2} + \frac{1}{2} \sum_{i \neq j} \sum_{\mathcal{J}_3\mathcal{J}_4\mathcal{J}_5\mathcal{J}_6} V^{ij}_{\mathcal{J}_3\mathcal{J}_4\mathcal{J}_5\mathcal{J}_6} D^i_{\mathcal{J}_3\mathcal{J}_6} D^j_{\mathcal{J}_4\mathcal{J}_5} \, . \tag{4.32}$$

The operators $D^i_{\mathcal{J}_1\mathcal{J}_2}$ satisfy the commutation relations

$$\left[D^i_{\mathcal{J}_1\mathcal{J}_2}, D^j_{\mathcal{J}_3\mathcal{J}_4} \right] = \delta_{ij} \left[\delta_{\mathcal{J}_2\mathcal{J}_3} D^i_{\mathcal{J}_1\mathcal{J}_4} - \delta_{\mathcal{J}_1\mathcal{J}_4} D^i_{\mathcal{J}_3\mathcal{J}_2} \right] \, . \tag{4.33}$$

Considering only the low lying eigenstates $|\psi_n\rangle$ and neglecting the overlap we can also use the following effective properties

$$\sum_{\mathcal{J}} D^{\imath}_{\mathcal{J}\mathcal{J}} = 1 \tag{4.34}$$

and

$$D^{\imath}_{\mathcal{J}_1\mathcal{J}_2} D^{\imath}_{\mathcal{J}_3\mathcal{J}_4} = \delta_{\mathcal{J}_2\mathcal{J}_3} D^{\imath}_{\mathcal{J}_1\mathcal{J}_4} \,. \tag{4.35}$$

Wigner's result follows directly by choosing the ground state $|\psi_0\rangle$ equal to $|\Psi_{HF}\rangle$ as given in (3.7). Then the ground state energy is approximated by

$$\begin{aligned} E_0 &= \langle \Psi_{HF} | H_{\text{eff}} | \Psi_{HF} \rangle = 2N\, T_{00} + \frac{1}{2} \sum_{\imath \neq \jmath} V^{\imath\jmath}_{0000} \\ &= 2N \frac{3\hbar^2}{8m\alpha} + \frac{1}{2} \sum_{\imath \neq \jmath} \sum_{\boldsymbol{q}}{}' \frac{4\pi e^2}{\Omega q^2} e^{-\alpha q^2} \exp[i\boldsymbol{q} \cdot \boldsymbol{R}_{\imath\jmath}] \,. \end{aligned} \tag{4.36}$$

Minimizing E_0 with respect to α and neglecting all terms containing erfc $\left(\frac{R_{\imath\jmath}}{2\sqrt{\alpha}}\right)$ leads to Wigner's ground state energy.

In order to take into account the electron-electron correlation we substitute first

$$L^{(\boldsymbol{\ell}_> - \boldsymbol{\ell}_<)\cdot\hat{\boldsymbol{\xi}}}_{\boldsymbol{\ell}_<\cdot\hat{\boldsymbol{\xi}}} (\alpha(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^2) = \sum_{m=0}^{\boldsymbol{\ell}_<\cdot\hat{\boldsymbol{\xi}}} (-1)^m \begin{pmatrix} \boldsymbol{\ell}_> \cdot \hat{\boldsymbol{\xi}} \\ \boldsymbol{\ell}_< \cdot \hat{\boldsymbol{\xi}} - m \end{pmatrix} \frac{[\alpha(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^2]^m}{m!} \tag{4.37}$$

into the matrix elements $V^{\imath\jmath}_{\mathcal{J}_3\mathcal{J}_4\mathcal{J}_5\mathcal{J}_6}$. As shown in appendix V that leads to the following expression for the interaction operator V of an electron lattice with cubic symmetry:

$$\begin{aligned} V &= E_{Cl} + \frac{1}{2} \sum_{\imath \neq \jmath} \sum_{\boldsymbol{q}}{}' e^{i\boldsymbol{q}\cdot\boldsymbol{R}_{\imath\jmath}} \frac{4\pi e^2}{\Omega q^2} e^{-\alpha q^2} \left\{ \frac{1}{2} \alpha \left[i\boldsymbol{q} \cdot (\boldsymbol{S}_\imath - \boldsymbol{S}_\jmath) \right]^2 \right. \\ &+ \left. \frac{1}{6} \alpha\sqrt{\alpha} \left[i\boldsymbol{q} \cdot (\boldsymbol{S}_\imath - \boldsymbol{S}_\jmath) \right]^3 + \frac{1}{24} \alpha^2 \left[i\boldsymbol{q} \cdot (\boldsymbol{S}_\imath - \boldsymbol{S}_\jmath) \right]^4 \right\} \,, \end{aligned} \tag{4.38}$$

where terms containing q^n, $n > 4$, are neglected and the operators $\boldsymbol{S}_\imath$ are given by

$$\boldsymbol{S}_\imath = \sum_{\hat{\boldsymbol{\xi}}} \hat{\boldsymbol{\xi}}\, S^{\imath}_{\hat{\boldsymbol{\xi}}} \tag{4.39}$$

with

$$S^{\imath}_{\hat{\boldsymbol{\xi}}} = \sum_{\mathcal{J}} \sqrt{\mathcal{J}\cdot\hat{\boldsymbol{\xi}} + 1}\, [D^{\imath}_{\mathcal{J}+\hat{\boldsymbol{\xi}},\mathcal{J}} + D^{\imath}_{\mathcal{J},\mathcal{J}+\hat{\boldsymbol{\xi}}}] \,. \tag{4.40}$$

Now $H_{\rm eff}$ can be treated exactly up to order $(\boldsymbol{S}_\imath - \boldsymbol{S}_\jmath)^2$. In that case the relevant interaction operator reads

$$V = E_{CI} + \frac{1}{2} \sum_{\imath \neq \jmath} \sum_{\boldsymbol{q}}{}' e^{\imath \boldsymbol{q} \cdot \boldsymbol{R}_{\imath\jmath}} \frac{4\pi e^2}{\Omega q^2} e^{-\alpha q^2} \sum_{\hat{\boldsymbol{\xi}}, \hat{\boldsymbol{\eta}}} \alpha (\boldsymbol{q} \cdot \hat{\boldsymbol{\xi}})(\boldsymbol{q} \cdot \hat{\boldsymbol{\eta}}) \left[S^\imath_{\hat{\boldsymbol{\xi}}} S^\jmath_{\hat{\boldsymbol{\eta}}} - \frac{1}{2} S^\imath_{\hat{\boldsymbol{\xi}}} S^\imath_{\hat{\boldsymbol{\eta}}} - \frac{1}{2} S^\jmath_{\hat{\boldsymbol{\xi}}} S^\jmath_{\hat{\boldsymbol{\eta}}} \right] , \tag{4.41}$$

with

$$\begin{aligned} &\sum_{\boldsymbol{q}}{}' e^{\imath \boldsymbol{q} \cdot \boldsymbol{R}_{\imath\jmath}} \frac{4\pi e^2}{\Omega q^2} e^{-\alpha q^2} (\boldsymbol{q} \cdot \hat{\boldsymbol{\xi}})(\boldsymbol{q} \cdot \hat{\boldsymbol{\eta}}) = \\ &\quad -e^2 \left[\delta_{\hat{\boldsymbol{\xi}}\hat{\boldsymbol{\eta}}} \left(\frac{\exp(-R_{\imath\jmath}^2/4\alpha)}{\sqrt{\pi\alpha}\, R_{\imath\jmath}^2} + \frac{\operatorname{erfc}(R_{\imath\jmath}/2\sqrt{\alpha})}{R_{\imath\jmath}^3} - \frac{1}{R_{\imath\jmath}^3} \right) \right. \\ &\quad \left. + (\boldsymbol{R}_{\imath\jmath} \cdot \hat{\boldsymbol{\xi}})(\boldsymbol{R}_{\imath\jmath} \cdot \hat{\boldsymbol{\eta}}) \left[\frac{3}{R_{\imath\jmath}^5} - \frac{3 \operatorname{erfc}(R_{\imath\jmath}/2\sqrt{\alpha})}{R_{\imath\jmath}^5} - \frac{\exp(-R_{\imath\jmath}^2/4\alpha)}{R_{\imath\jmath}^2} \left(\frac{1}{2\alpha\sqrt{\pi\alpha}} + \frac{3}{R_{\imath\jmath}^2 \sqrt{\pi\alpha}} \right) \right] \right] \end{aligned} \tag{4.42}$$

and

$$\frac{1}{2} \sum_{\boldsymbol{R}_\imath \neq 0} \sum_{\boldsymbol{q}}{}' e^{\imath \boldsymbol{q} \cdot \boldsymbol{R}_\imath} \frac{4\pi e^2}{\Omega q^2} e^{-\alpha q^2} (\boldsymbol{q} \cdot \hat{\boldsymbol{\xi}})(\boldsymbol{q} \cdot \hat{\boldsymbol{\eta}}) = \delta_{\hat{\boldsymbol{\xi}}\hat{\boldsymbol{\eta}}} \left[\frac{-4\pi N e^2}{3\Omega} + \sum_{\boldsymbol{R}_\imath \neq 0} e^{-R_\imath^2/4\alpha} \frac{e^2}{12\alpha\sqrt{\pi\alpha}} \right] , \tag{4.43}$$

where use is made of the cubic symmetry of the lattice in the last calculation. Neglecting the terms in (4.42) and (4.43) of the order of the overlap, i.e. terms containing $\exp(-R_{\imath\jmath}^2/4\alpha)$ and $\operatorname{erfc}(R_{\imath\jmath}/2\sqrt{\alpha})$, we arrive at

$$V = E_{CI} + \frac{1}{2} \alpha \sum_{\imath,\jmath} \sum_{\hat{\boldsymbol{\xi}}, \hat{\boldsymbol{\eta}}} M_{\hat{\boldsymbol{\xi}}\hat{\boldsymbol{\eta}}}(\boldsymbol{R}_{\imath\jmath})\, S^\imath_{\hat{\boldsymbol{\xi}}} S^\jmath_{\hat{\boldsymbol{\eta}}} , \tag{4.44}$$

where the elements of the second rank tensor $\boldsymbol{M}(\boldsymbol{R}_{\imath\jmath})$ are given by

$$\begin{aligned} M_{\hat{\boldsymbol{\xi}}\hat{\boldsymbol{\eta}}}(\boldsymbol{R}_{\imath\jmath}) &= e^2 \left[\frac{1}{R_{\imath\jmath}^3} \delta_{\hat{\boldsymbol{\xi}}\hat{\boldsymbol{\eta}}} - \frac{3}{R_{\imath\jmath}^5} (\boldsymbol{R}_{\imath\jmath} \cdot \hat{\boldsymbol{\xi}})(\boldsymbol{R}_{\imath\jmath} \cdot \hat{\boldsymbol{\eta}}) \right] , \quad \text{for } \imath \neq \jmath , \\ M_{\hat{\boldsymbol{\xi}}\hat{\boldsymbol{\eta}}}(0) &= \frac{8\pi N e^2}{3\Omega} \delta_{\hat{\boldsymbol{\xi}}\hat{\boldsymbol{\eta}}} . \end{aligned} \tag{4.45}$$

These tensor elements are identical to the elements $M(\boldsymbol{R}_{\imath\jmath})_{\mu\nu}$, with $\mu, \nu = x, y, z$, as given by (4.2).

The kinetic energy term T reads according to (4.28) and (4.32):

$$T = \frac{\hbar^2}{4m\alpha} \sum_{\iota} \sum_{\hat{\boldsymbol{\xi}}} \sum_{\boldsymbol{\jmath}} \left[(\frac{1}{2} + \boldsymbol{\jmath} \cdot \hat{\boldsymbol{\xi}}) D^{\iota}_{\boldsymbol{\jmath}\boldsymbol{\jmath}} - \frac{1}{2} \sqrt{(\boldsymbol{\jmath} \cdot \hat{\boldsymbol{\xi}} + 1)(\boldsymbol{\jmath} \cdot \hat{\boldsymbol{\xi}} + 2)} \, (D^{i}_{\boldsymbol{\jmath}\boldsymbol{\jmath}+2\hat{\boldsymbol{\xi}}} + D^{\iota}_{\boldsymbol{\jmath}+2\hat{\boldsymbol{\xi}}\boldsymbol{\jmath}}) \right] . \tag{4.46}$$

Introducing the operators

$$P^{\iota}_{\hat{\boldsymbol{\xi}}} = \sum_{\boldsymbol{\jmath}} \sqrt{\boldsymbol{\jmath} \cdot \hat{\boldsymbol{\xi}} + 1} \, [D^{\iota}_{\boldsymbol{\jmath}\boldsymbol{\jmath}+\hat{\boldsymbol{\xi}}} - D^{i}_{\boldsymbol{\jmath}+\hat{\boldsymbol{\xi}}\boldsymbol{\jmath}}] , \tag{4.47}$$

we obtain using (4.35):

$$T = -\frac{\hbar^2}{8m\alpha} \sum_{i,\hat{\boldsymbol{\xi}}} P^{\iota}_{\hat{\boldsymbol{\xi}}} P^{\iota}_{\hat{\boldsymbol{\xi}}} . \tag{4.48}$$

Thus H_{eff} can be expressed as the following bilinear form:

$$H_{\text{eff}} = -\frac{\hbar^2}{8m\alpha} \sum_{i,\hat{\boldsymbol{\xi}}} P^{\iota}_{\hat{\boldsymbol{\xi}}} P^{\iota}_{\hat{\boldsymbol{\xi}}} + E_{Cl} + \frac{1}{2} \alpha \sum_{\iota,\jmath} \sum_{\hat{\boldsymbol{\xi}},\hat{\boldsymbol{\eta}}} M_{\hat{\boldsymbol{\xi}}\hat{\boldsymbol{\eta}}}(\boldsymbol{R}_{\iota\jmath}) S^{\iota}_{\hat{\boldsymbol{\xi}}} S^{\jmath}_{\hat{\boldsymbol{\eta}}} . \tag{4.49}$$

In order to determine the eigenvalues of H_{eff} we make use of the commutator

$$[P^{\iota}_{\hat{\boldsymbol{\xi}}}, S^{\jmath}_{\hat{\boldsymbol{\eta}}}] = \delta_{\iota\jmath}\delta_{\hat{\boldsymbol{\xi}}\hat{\boldsymbol{\eta}}} \sum_{\boldsymbol{\jmath}} 2D^{\iota}_{\boldsymbol{\jmath}\boldsymbol{\jmath}} = 2\delta_{\iota\jmath}\delta_{\hat{\boldsymbol{\xi}}\hat{\boldsymbol{\eta}}} , \tag{4.50}$$

which holds because of (4.33) and (4.34). Then H_{eff} can be diagonalized analogous to Carr's procedure. Introducing

$$\begin{aligned} S_{\boldsymbol{k}\lambda} &= \frac{1}{\sqrt{2N}} \sum_{i,\hat{\boldsymbol{\xi}}} e^{-i\boldsymbol{k} \cdot \boldsymbol{R}_{\iota}} \boldsymbol{\varepsilon}_{-\boldsymbol{k}\lambda} \cdot \hat{\boldsymbol{\xi}} \, S^{\iota}_{\hat{\boldsymbol{\xi}}} , \\ P_{\boldsymbol{k}\lambda} &= \frac{1}{\sqrt{2N}} \sum_{i,\hat{\boldsymbol{\xi}}} e^{i\boldsymbol{k} \cdot \boldsymbol{R}_{\iota}} \boldsymbol{\varepsilon}_{\boldsymbol{k}\lambda} \cdot \hat{\boldsymbol{\xi}} \, P^{\iota}_{\hat{\boldsymbol{\xi}}} \end{aligned} \tag{4.51}$$

we arrive at

$$H_{\text{eff}} = E_{Cl} - \frac{\hbar^2}{8m\alpha} \sum_{\boldsymbol{k}\lambda} P_{\boldsymbol{k}\lambda} P_{-\boldsymbol{k}\lambda} + \frac{1}{2} \alpha \sum_{\boldsymbol{k}\lambda} m\omega^2_{\boldsymbol{k}\lambda} S_{-\boldsymbol{k}\lambda} S_{\boldsymbol{k}\lambda} , \tag{4.52}$$

where $\boldsymbol{\varepsilon}_{\boldsymbol{k}\lambda}$ and $\omega_{\boldsymbol{k}\lambda}$ are given by the eigenvalue equation (4.4). The operators $S_{\boldsymbol{k}\lambda}$ and $P_{\boldsymbol{k}\lambda}$ satisfy

$$\begin{aligned} [S_{\boldsymbol{k}\lambda}, S_{\boldsymbol{k}'\lambda'}] &= [P_{\boldsymbol{k}\lambda}, P_{\boldsymbol{k}'\lambda'}] = 0 , \\ [P_{\boldsymbol{k}\lambda}, S_{\boldsymbol{k}'\lambda'}] &= \frac{1}{2N} \sum_{i,\boldsymbol{\jmath}} 2D^{\iota}_{\boldsymbol{\jmath}\boldsymbol{\jmath}} e^{i(\boldsymbol{k}-\boldsymbol{k}')\boldsymbol{R}_{\iota}} \boldsymbol{\varepsilon}_{\boldsymbol{k}\lambda} \cdot \boldsymbol{\varepsilon}_{-\boldsymbol{k}'\lambda'} = 2\delta_{\boldsymbol{k}\boldsymbol{k}'}\delta_{\lambda\lambda'} . \end{aligned} \tag{4.53}$$

The effective Hamiltonian (4.52) can be rewritten in terms of the boson operators

$$A_{\boldsymbol{k}\lambda} = \sqrt{\frac{m\omega_{\boldsymbol{k}\lambda}\alpha}{2\hbar}}\, S_{\boldsymbol{k}\lambda} + \sqrt{\frac{\hbar}{8m\omega_{\boldsymbol{k}\lambda}\alpha}}\, P_{-\boldsymbol{k}\lambda} \,,$$
$$A^{+}_{\boldsymbol{k}\lambda} = \sqrt{\frac{m\omega_{\boldsymbol{k}\lambda}\alpha}{2\hbar}}\, S_{-\boldsymbol{k}\lambda} - \sqrt{\frac{\hbar}{8m\omega_{\boldsymbol{k}\lambda}\alpha}}\, P_{\boldsymbol{k}\lambda} \,, \tag{4.54}$$

that satisfy the commutation relations

$$\begin{aligned} [A_{\boldsymbol{k}\lambda}, A_{\boldsymbol{k}'\lambda'}] &= [A^{+}_{\boldsymbol{k}\lambda},\ A^{+}_{\boldsymbol{k}'\lambda'}] = 0 \,, \\ [A_{\boldsymbol{k}\lambda}, A^{+}_{\boldsymbol{k}'\lambda'}] &= \delta_{\boldsymbol{k}\boldsymbol{k}'}\delta_{\boldsymbol{\lambda}\lambda'} \,. \end{aligned} \tag{4.55}$$

Then the effective Hamiltonian is

$$H_{\text{eff}} = E_{Cl} + \sum_{\boldsymbol{k}\lambda} \hbar\omega_{\boldsymbol{k}\lambda}\,[\frac{1}{2} + A^{+}_{\boldsymbol{k}\lambda}A_{\boldsymbol{k}\lambda}] \,. \tag{4.56}$$

The corresponding internal energy is given by

$$E = E_{Cl} + \sum_{\boldsymbol{k}\lambda} \left[\frac{1}{2} + \frac{1}{\exp(\beta\hbar\omega_{\boldsymbol{k}\lambda}) - 1}\right] \hbar\omega_{\boldsymbol{k}\lambda} \,, \tag{4.57}$$

where $\beta = \frac{1}{k_B T}$ with k_B and T denoting the Boltzmann constant and temperature, respectively.

As to the internal energy (4.57) the following remarks should be made. First of all it only holds provided that exchange terms can be neglected. Such an approximation is only valid for the low density electron system at low temperatures. For the statistical weight of the higher excited states $|\psi_n\rangle$ increases with temperature, meaning that even at low density the overlap is not negligible at higher temperatures. The ground state energy is exact up to order $r_s^{-3/2}$. The terms of order $(\boldsymbol{S}_i - \boldsymbol{S}_j)^n$, $n > 2$, which were also neglected, can be dealt with as a perturbation and give rise to terms of the order of $r_s^{-2}, r_s^{-5/2}, r_s^{-3}, \ldots$ in the ground state energy (see Appendix V).

Carr's approach and ours become mathematically identical when identifying $\boldsymbol{r}_i - \boldsymbol{R}_i$ with $\sqrt{\alpha}\,\boldsymbol{S}_i$ and $a^{(+)}_{\boldsymbol{k}\lambda}$ with $A^{(+)}_{\boldsymbol{k}\lambda}$. That identity does not only hold for Carr's harmonic term and our $(\boldsymbol{S}_i - \boldsymbol{S}_j)^2$ term but also for his anharmonic terms and our corresponding

$(\boldsymbol{S}_i - \boldsymbol{S}_j)^n$ terms. Consequently the energy terms of order r_s^{-2}, $r_s^{-5/2}$, r_s^{-3},... can be calculated according to the theory of anharmonic lattices [11],[12],[13].

Finally we discuss the already mentioned epistomological questions arising from the semiclassical nature of Carr's approach.

(1) Carr's results can be obtained indeed in a fully quantummechanical way. Although the terms of our effective Hamiltonian and the corresponding ones of Carr's expansion can be treated in a mathematically identical way, the present approach does not break the permutation symmetry. Therefore our effective Hamiltonian cannot result from Carr's expansion.

(2) The low density electron system can indeed be effectively described up to order $r_s^{-3/2}$ in terms of a system of free bosons, provided that exchange is neglected. The appearing boson operators $A^{(+)}_{\boldsymbol{k}\lambda}$ are bilinear expressions of the original fermion operators as follows from (4.31), (4.40), (4.47), (4.51) and (4.54).

(3) The ground state $|\psi_0\rangle$ of the effective Hamiltonian (4.56) is obtained by requiring

$$A_{\boldsymbol{k}\lambda}|\psi_0\rangle = 0\ , \tag{4.58}$$

for all $\boldsymbol{k}$ and λ. As shown in Appendix VI the requirement (4.58) gives rise to relations between the coefficients $A^{\sigma_1,\ \ldots\ \sigma_{2N}}_{j_1,\ \ldots\ j_{2N}}(0)$ of the decomposition (4.13) that completely determine $|\psi_0\rangle$. It should be remarked here that the correlated ground state $|\psi_0\rangle$ still depends on a seemingly free parameter α. However, although the energy (4.57) does not depend on α, the choice of α is restricted by the requirement that overlap must be negligible for large r_s. This means that the width $\alpha^{1/2}$ of the harmonic oscillator wave functions must be small compared with the nearest neighbour distance.

5. The effect of a magnetic field on the Wigner lattice

A detailed study of the properties of the three-dimensional low-density electron system in the presence of a magnetic field has never been published, as far as we know. The results as obtained by Fukuyama [14], [15] and Fukuyama and McClure [16] in their study of the two-dimensional case with the field perpendicular to the lattice plane cannot be simply generalized to three dimensions. For the macroscopic magnetic field is no longer the applied external field but an internal field, that must be determined selfconsistently. This is done as follows. First an Ansatz is chosen for the magnetic field. Next the response of the system to that field is calculated. Then the internal field is calculated by means of Maxwell's equations with the response as source term and compared with the Ansatz. In case of difference the procedure is repeated starting from the calculated field, until selfconsistency is obtained.

In part A of this section we use the described procedure to show that the low-density jellium model allows a homogeneous internal field. Besides the effect of this field on the ground state energy of the Wigner lattice is calculated exactly up to order $r_s^{-3/2}$. The strength of the internal field cannot be calculated as boundary conditions are absent here. This means that it is unclear whether a field can actually penetrate into the system. For that reason we pay, in part B, attention to the effect of boundary conditions by considering the response to an inhomogeneous field. It appears that the system does not show the Meissner-Ochsenfeld effect, i.e. the field does penetrate the system.

A. Homogeneous magnetic field

In order to show that the jellium model allows a homogeneous magnetic field we take a constant internal field $B = B\hat{z}$ as an Ansatz. The jellium model in the presence of such a field is described in terms of the Hamiltonian

$$H = \sum_{\sigma} \int d^3r\, \psi_\sigma^+(\boldsymbol{r}) \left[\frac{\hbar}{i} \nabla - \frac{e}{c} \boldsymbol{A}(\boldsymbol{r}) \right]^2 \frac{1}{2m} \psi_\sigma(\boldsymbol{r})$$

$$+ \frac{1}{2} \sum_{\boldsymbol{q}}{}' \sum_{\boldsymbol{k},\boldsymbol{k}'} \sum_{\sigma,\sigma'} V(\boldsymbol{q}) c^{+}_{\boldsymbol{k}\sigma} c^{+}_{\boldsymbol{k}'\sigma'} c_{\boldsymbol{k}'+\boldsymbol{q}\sigma'} c_{\boldsymbol{k}-\boldsymbol{q}\sigma}$$

$$- \mu_B B \sum_{\boldsymbol{k}} [c^{+}_{\boldsymbol{k}\uparrow} c_{\boldsymbol{k}\uparrow} - c^{+}_{\boldsymbol{k}\downarrow} c_{\boldsymbol{k}\downarrow}] \tag{5.1}$$

where $\boldsymbol{A}$ is the vector potential defined by $\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}$ and μ_B is the Bohr magneton $\frac{e\hbar}{2mc}$. The last term in (5.1) describes the interaction of the electron spins with the magnetic field. The vector potential is chosen according to the symmetric gauge:

$$\boldsymbol{A}(\boldsymbol{r}) = \frac{1}{2} \boldsymbol{B} \times \boldsymbol{r} = \frac{1}{2} B[x\hat{\boldsymbol{y}} - y\hat{\boldsymbol{x}}] \,. \tag{5.2}$$

In order to calculate the energy spectrum and the low-lying eigenstates of the Hamiltonian (5.1) up to order $r_s^{-3/2}$ the procedure of section 4 is followed. The underlying assumption is that a small magnetic field does not destroy the Wigner lattice, i.e. the effect of exchange on the energies of the low-lying eigenstates is negligible for low densities. The behaviour of the quantummechanical Wigner lattice is analogous to that of the classical lattice. Thus we can choose the positions of the lattice to be time-independent. It should be noted that the situation is quite different for an electric field. For each site $\boldsymbol{R}_i$, $i = 1, \ldots, 2N$, a complete set of one-electron functions that depend on the magnetic field B and the lattice site $\boldsymbol{R}_i$ is chosen. These functions $f^{B}_{\boldsymbol{\jmath}\boldsymbol{R}_i}$ are localized at $\boldsymbol{R}_i$ in such a way that their mutual overlap can be neglected for small $|\boldsymbol{\jmath}|$.

The eigenstates of (5.1) can be written as (cf. (4.13))

$$|\psi^{B}_{n}\rangle = \sum_{\substack{\boldsymbol{\jmath}_1, \ldots, \boldsymbol{\jmath}_{2N} \\ \sigma_1, \ldots, \sigma_{2N}}} A^{\sigma_1 \ldots \sigma_{2N}}_{\boldsymbol{\jmath}_1 \ldots \boldsymbol{\jmath}_{2N}}(B, n)\, d^{+}_{B\boldsymbol{\jmath}_1\sigma_1}(\boldsymbol{R}_1) \ldots d^{+}_{B\boldsymbol{\jmath}_{2N}\sigma_{2N}}(\boldsymbol{R}_{2N})|\rangle \,, \tag{5.3}$$

where the fermion operators $d^{+}_{B\boldsymbol{\jmath}_i\sigma_i}(\boldsymbol{R}_i)$ are defined as

$$\begin{aligned} d^{+}_{B\boldsymbol{\jmath}_i\sigma_i}(\boldsymbol{R}_i) &= \int d^3r\, \psi^{+}_{\sigma_i}(\boldsymbol{r}) f^{B}_{\boldsymbol{\jmath}_i\boldsymbol{R}_i}(\boldsymbol{r} - \boldsymbol{R}_i) \\ &= \left[\frac{(2\pi)^3}{\Omega}\right]^{1/2} \sum_{\boldsymbol{k}} \exp[-i\boldsymbol{k} \cdot \boldsymbol{R}_i] \hat{f}^{B}_{\boldsymbol{\jmath}_i\boldsymbol{R}_i}(\boldsymbol{k}) c^{+}_{\boldsymbol{k}\sigma_i} \,, \end{aligned} \tag{5.4}$$

with $\hat{f}^B_{\mathcal{J}_1 \boldsymbol{R}_\imath}$ being the Fourier transform of $f^B_{\mathcal{J}_1 \boldsymbol{R}_\imath}$.

Because the effect of exchange is neglected for low densities and low temperatures in a first approximation we can replace the original Hamiltonian (5.1) by the following effective Hamiltonian:

$$\begin{aligned} H_{\text{eff}} &= \sum_{\imath} \sum_{\mathcal{J}_1 \mathcal{J}_2 \sigma} T^{\imath}_{B \mathcal{J}_1 \mathcal{J}_2} \, d^+_{B \mathcal{J}_1 \sigma}(\boldsymbol{R}_\imath) d_{B \mathcal{J}_2 \sigma}(\boldsymbol{R}_\imath) \\ &+ \frac{1}{2} \sum_{\imath \neq \jmath} \sum_{\mathcal{J}_3 \mathcal{J}_4 \mathcal{J}_5 \mathcal{J}_6, \sigma, \sigma'} V^{\imath\jmath}_{B \mathcal{J}_3 \mathcal{J}_4 \mathcal{J}_5 \mathcal{J}_6} \, d^+_{B \mathcal{J}_3 \sigma}(\boldsymbol{R}_\imath) \, d^+_{B \mathcal{J}_4 \sigma'}(\boldsymbol{R}_\jmath) \, d_{B \mathcal{J}_5 \sigma'}(\boldsymbol{R}_\jmath) \, d_{B \mathcal{J}_6 \sigma}(\boldsymbol{R}_\imath) \\ &- \mu_B B \sum_{\imath} \sum_{\mathcal{J}_7 \mathcal{J}_8} U^{\imath}_{B \mathcal{J}_7 \mathcal{J}_8} [d^+_{B \mathcal{J}_7 \uparrow}(\boldsymbol{R}_\imath) \, d_{B \mathcal{J}_8 \uparrow}(\boldsymbol{R}_\imath) - d^+_{B \mathcal{J}_7 \downarrow}(\boldsymbol{R}_\imath) \, d_{B \mathcal{J}_8 \downarrow}(\boldsymbol{R}_\imath)] \, , \end{aligned} \tag{5.5}$$

where

$$T^{\imath}_{B \mathcal{J}_1 \mathcal{J}_2} = \int d^3 r \, f^B_{\mathcal{J}_1 \boldsymbol{R}_\imath}(\boldsymbol{r} - \boldsymbol{R}_\imath) \left[\frac{\hbar}{i} \nabla - \frac{eB}{2c} (x \hat{\boldsymbol{y}} - y \hat{\boldsymbol{x}}) \right]^2 \frac{1}{2m} f^{*B}_{\mathcal{J}_2 \boldsymbol{R}_\imath}(\boldsymbol{r} - \boldsymbol{R}_\imath) \, , \tag{5.6}$$

$$V^{\imath\jmath}_{B \mathcal{J}_3 \mathcal{J}_4 \mathcal{J}_5 \mathcal{J}_6} = \sum_{\boldsymbol{q}}{}' \frac{4\pi e^2}{\Omega q^2} \, e^{i \boldsymbol{q} \cdot \boldsymbol{R}_{\imath\jmath}} \int d^3 k \, d^3 k' \, \hat{f}^B_{\mathcal{J}_3 \boldsymbol{R}_\imath}(\boldsymbol{k}) \, \hat{f}^B_{\mathcal{J}_4 \boldsymbol{R}_\jmath}(\boldsymbol{k}') \, \hat{f}^{*B}_{\mathcal{J}_5 \boldsymbol{R}_\jmath}(\boldsymbol{k}' + \boldsymbol{q}) \, \hat{f}^{*B}_{\mathcal{J}_6 \boldsymbol{R}_\imath}(\boldsymbol{k} - \boldsymbol{q}) \tag{5.7}$$

and

$$U^{\imath}_{B \mathcal{J}_7 \mathcal{J}_8} = \int d^3 k \, \hat{f}^B_{\mathcal{J}_7 \boldsymbol{R}_\imath}(\boldsymbol{k}) \hat{f}^{*B}_{\mathcal{J}_8 \boldsymbol{R}_\imath}(\boldsymbol{k}) \, . \tag{5.8}$$

Clearly the low-lying states of H_{eff} and their attendant energies do not depend on the choice of the functions $f^B_{\mathcal{J} \boldsymbol{R}_\imath}$ as these functions are chosen to satisfy the following requirements:

(1) They must form a complete set for each lattice site $\boldsymbol{R}_\imath$.

(2) Their mutual overlap must be negligible for small $|\mathcal{J}|$.

As will be shown a very convenient choice is

$$f^B_{\mathcal{J} \boldsymbol{R}_\imath}(\boldsymbol{r} - \boldsymbol{R}_\imath) = \exp \left[i \boldsymbol{R}_\imath \frac{eB}{2c\hbar} (y \hat{\boldsymbol{x}} - x \hat{\boldsymbol{y}}) \right] f_{\mathcal{J}}(\boldsymbol{r} - \boldsymbol{R}_\imath) \, , \tag{5.9}$$

where $f_{\mathcal{J}}$ is the harmonic oscillator eigenfunction (4.12). Then the Fourier transform is given by

$$\hat{f}^B_{\mathcal{J} \boldsymbol{R}_\imath}(\boldsymbol{k}) = \hat{f}_{\mathcal{J}} \left(\boldsymbol{k} - \frac{e}{2c\hbar} [\boldsymbol{R}_\imath \times \boldsymbol{B}] \right) \, , \tag{5.10}$$

with $\hat{f}_{\mathcal{J}}$ being the Fourier transform (4.15) of the function (4.12). The functions (5.9) have the required properties as can easily be checked.

(1) They form a complete set as follows from the completeness of the harmonic oscillator eigenfunctions.

(2) The overlap between functions localized around different lattice sites $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$ is given by (cf. (4.16))

$$\begin{aligned} S^B_{\mathcal{J}_1\mathcal{J}_2}(\boldsymbol{R}_{12}) &= \int d^3r\, f^{*B}_{\mathcal{J}_1\boldsymbol{R}_1}(\boldsymbol{r}-\boldsymbol{R}_1) f^B_{\mathcal{J}_2\boldsymbol{R}_2}(\boldsymbol{r}-\boldsymbol{R}_2) \\ &= \exp\left[\frac{-R_{12}^2}{8\alpha} - \frac{1}{2}\alpha\,[\boldsymbol{R}_{12}\times\frac{\boldsymbol{B}e}{2c\hbar}]^2\right] \prod_{\hat{\boldsymbol{\xi}}} \left[\frac{2^{\mathcal{J}_>\cdot\hat{\boldsymbol{\xi}}}(\mathcal{J}_<\cdot\hat{\boldsymbol{\xi}})!}{2^{\mathcal{J}_<\hat{\boldsymbol{\xi}}}(\mathcal{J}_>\cdot\hat{\boldsymbol{\xi}})!}\right]^{1/2} \\ &\times \left[\left(\frac{\boldsymbol{R}_{12}\cdot\hat{\boldsymbol{\xi}} + 2\imath\alpha[\boldsymbol{R}_{12}\times\boldsymbol{B}e/2c\hbar]\cdot\hat{\boldsymbol{\xi}}}{2\sqrt{2\alpha}}\right)^{(\mathcal{J}_>-\mathcal{J}_<)\hat{\boldsymbol{\xi}}}\right. \\ &\times \left. L^{(\mathcal{J}_>-\mathcal{J}_<)\hat{\boldsymbol{\xi}}}_{\mathcal{J}_<\hat{\boldsymbol{\xi}}}\left(\frac{(\boldsymbol{R}_{12}\cdot\hat{\boldsymbol{\xi}})^2 + 4\alpha^2([\boldsymbol{R}_{12}\times\boldsymbol{B}e/2c\hbar]\cdot\hat{\boldsymbol{\xi}})^2}{4\alpha}\right)\right], \end{aligned} \tag{5.11}$$

and can indeed be neglected at low densities for small $|\mathcal{J}_1|$ and $|\mathcal{J}_2|$.

Now the reason for our choice of the functions $f^B_{\mathcal{J}\boldsymbol{R}_i}$ is clear. For the matrix elements $T^i_{B\mathcal{J}_1\mathcal{J}_2}$ do not depend on $\boldsymbol{R}_i$ due to the phase factor in (5.9). Further the factor does not appear in the matrix elements $V^{ij}_{B\mathcal{J}_3\mathcal{J}_4\mathcal{J}_5\mathcal{J}_6}$ and $U^i_{B\mathcal{J}_7\mathcal{J}_8}$ as well. Substitution of (5.9) and (5.10) into (5.6), (5.7) and (5.8), respectively, gives

$$\begin{aligned} T_{B\mathcal{J}_1\mathcal{J}_2} &= \int d^3r\, f_{\mathcal{J}_1}(\boldsymbol{r})\left[\frac{\hbar}{i}\nabla - \frac{eB}{2c}(x\hat{\boldsymbol{y}} - y\hat{\boldsymbol{x}})\right]^2 \frac{1}{2m} f^*_{\mathcal{J}_2}(\boldsymbol{r}) \\ &= \sum_{\hat{\boldsymbol{\xi}}\in\{\hat{\boldsymbol{x}},\hat{\boldsymbol{y}},\hat{\boldsymbol{z}}\}} \frac{\hbar^2}{4m\alpha}\left[\delta_{\mathcal{J}_1\mathcal{J}_2}(\mathcal{J}_1\cdot\hat{\boldsymbol{\xi}} + \frac{1}{2}) - \frac{1}{2}\delta_{\mathcal{J}_1,\mathcal{J}_2+2\hat{\boldsymbol{\xi}}}\sqrt{(\mathcal{J}_2\cdot\hat{\boldsymbol{\xi}}+1)(\mathcal{J}_2\cdot\hat{\boldsymbol{\xi}}+2)}\right. \\ &- \left.\frac{1}{2}\delta_{\mathcal{J}_2,\mathcal{J}_1+2\hat{\boldsymbol{\xi}}}\sqrt{(\mathcal{J}_1\cdot\hat{\boldsymbol{\xi}}+1)(\mathcal{J}_1\cdot\hat{\boldsymbol{\xi}}+2)}\right] \\ &+ \imath\mu_B B\left[\delta_{\mathcal{J}_1+\hat{\boldsymbol{x}},\mathcal{J}_2+\hat{\boldsymbol{y}}}\sqrt{(\mathcal{J}_1\cdot\hat{\boldsymbol{x}}+1)(\mathcal{J}_2\cdot\hat{\boldsymbol{y}}+1)}\right. \end{aligned}$$

$$- \delta_{\mathcal{J}_2+\hat{\boldsymbol{x}},\mathcal{J}_1+\hat{\boldsymbol{y}}}\sqrt{(\mathcal{J}_1\cdot\hat{\boldsymbol{y}}+1)(\mathcal{J}_2\cdot\hat{\boldsymbol{x}}+1)}\,\Big]$$

$$+ \mu_B^2 B^2 \frac{m\alpha}{\hbar^2}\sum_{\hat{\boldsymbol{\xi}}\in\{\hat{\boldsymbol{x}},\hat{\boldsymbol{y}}\}}\Big[\delta_{\mathcal{J}_1\mathcal{J}_2}(\mathcal{J}_1\cdot\hat{\boldsymbol{\xi}}+\frac{1}{2})+\frac{1}{2}\delta_{\mathcal{J}_1,\mathcal{J}_2+2\hat{\boldsymbol{\xi}}}\sqrt{(\mathcal{J}_2\cdot\hat{\boldsymbol{\xi}}+1)(\mathcal{J}_2\cdot\hat{\boldsymbol{\xi}}+2)}$$

$$+ \frac{1}{2}\delta_{\mathcal{J}_2,\mathcal{J}_1+2\hat{\boldsymbol{\xi}}}\sqrt{(\mathcal{J}_1\cdot\hat{\boldsymbol{\xi}}+1)(\mathcal{J}_1\cdot\hat{\boldsymbol{\xi}}+2)}\,\Big]\ , \tag{5.12}$$

$$V^{\prime\prime}_{B\mathcal{J}_3\mathcal{J}_4\mathcal{J}_5\mathcal{J}_6} = V^{\prime\prime}_{\mathcal{J}_3\mathcal{J}_4\mathcal{J}_5\mathcal{J}_6}\ , \tag{5.13}$$

$$U^{\prime}_{B\mathcal{J}_7\mathcal{J}_8} = \int d^3k\,\hat{f}_{\mathcal{J}_7}(\boldsymbol{k})\,\hat{f}^*_{\mathcal{J}_8}(\boldsymbol{k}) = \delta_{\mathcal{J}_7\mathcal{J}_8}\ . \tag{5.14}$$

The matrix elements (5.13) are given by (4.29).

In terms of the operators

$$D^{\prime}_{B\mathcal{J}_1\mathcal{J}_2} = \sum_{\sigma} d^{+}_{B\mathcal{J}_1\sigma}(\boldsymbol{R}_i)d_{B\mathcal{J}_2\sigma}(\boldsymbol{R}_i)\ , \tag{5.15}$$

and the operators $\sum_{B_i}$ defined by

$$\sum_{B_i} = \sum_{\mathcal{J}} d^{+}_{B\mathcal{J}\mathcal{T}}(\boldsymbol{R}_i)d_{B\mathcal{J}\mathcal{1}}(\boldsymbol{R}_i) \tag{5.16}$$

the effective Hamiltonian can be rewritten as

$$H_{\text{eff}} = \sum_{i,\mathcal{J}}\Big[\frac{\hbar^2}{4m\alpha}\sum_{\hat{\boldsymbol{\xi}}}\Big[(\mathcal{J}\cdot\hat{\boldsymbol{\xi}}+\frac{1}{2})D^{\prime}_{B\mathcal{J}\mathcal{J}}$$

$$- \frac{1}{2}\sqrt{(\mathcal{J}\cdot\hat{\boldsymbol{\xi}}+1)(\mathcal{J}\cdot\hat{\boldsymbol{\xi}}+2)}\,(D^{\prime}_{B\mathcal{J},\mathcal{J}+2\hat{\boldsymbol{\xi}}}+D^{\prime}_{B\mathcal{J}+2\hat{\boldsymbol{\xi}},\mathcal{J}})\Big]$$

$$+ i\mu_B B\Big[\sqrt{(\mathcal{J}\cdot\hat{\boldsymbol{y}}+1)(\mathcal{J}\cdot\hat{\boldsymbol{x}}+1)}\,(D^{\prime}_{B\mathcal{J}+\hat{\boldsymbol{y}},\mathcal{J}+\hat{\boldsymbol{x}}}-D^{\prime}_{B\mathcal{J}+\hat{\boldsymbol{x}},\mathcal{J}+\hat{\boldsymbol{y}}})\Big]$$

$$+ \mu_B^2 B^2\frac{m\alpha}{\hbar^2}\sum_{\hat{\boldsymbol{\xi}}\in\{\hat{\boldsymbol{x}},\hat{\boldsymbol{y}}\}}\Big[(\mathcal{J}\cdot\hat{\boldsymbol{\xi}}+\frac{1}{2})D^{\prime}_{B\mathcal{J}\mathcal{J}}$$

$$+ \quad \frac{1}{2}\sqrt{(\mathcal{J}\cdot\hat{\boldsymbol{\xi}}+1)(\mathcal{J}\cdot\hat{\boldsymbol{\xi}}+2)}\,(D^{\prime}_{B\mathcal{J},\mathcal{J}+2\hat{\boldsymbol{\xi}}} - D^{\prime}_{B\mathcal{J}+2\hat{\boldsymbol{\xi}},\mathcal{J}})\Big]\Big]$$

$$+ \quad \frac{1}{2}\sum_{i\neq j}\sum_{\mathcal{J}_3\mathcal{J}_4\mathcal{J}_5\mathcal{J}_6} V^{ij}_{\mathcal{J}_3\mathcal{J}_4\mathcal{J}_5\mathcal{J}_6}\, D^{i}_{B\mathcal{J}_3\mathcal{J}_6} D^{j}_{B\mathcal{J}_4\mathcal{J}_5} - \mu_B B \sum_{i}\left[\Sigma_{Bi}\,\Sigma^{+}_{Bi} - \Sigma^{+}_{Bi}\,\Sigma_{Bi}\right] , \tag{5.17}$$

where use has been made of (5.12), (5.13), (5.14) and the relation:

$$\Sigma^{+}_{Bi}\,\Sigma_{Bi} = \sum_{\mathcal{J}} d^{+}_{B\mathcal{J}\downarrow}(\boldsymbol{R}_i)\, d_{B\mathcal{J}\downarrow}(\boldsymbol{R}_i) . \tag{5.18}$$

This relation holds provided that only low-lying eigenstates $|\psi^{B}_{n}\rangle$ are considered and overlap is neglected. In that case we can also use

$$\begin{aligned} \{\Sigma^{+}_{Bi},\Sigma_{Bi}\} &= \sum_{\mathcal{J}} D^{i}_{B\mathcal{J}\mathcal{J}} = 1 \\ D^{i}_{B\mathcal{J}_1\mathcal{J}_2} D^{i}_{B\mathcal{J}_3\mathcal{J}_4} &= \delta_{\mathcal{J}_2\mathcal{J}_3}\, D^{i}_{B\mathcal{J}_1\mathcal{J}_4} . \end{aligned} \tag{5.19}$$

Further the operators (5.15) and (5.16) satisfy the following commutation and anticommutation relations:

$$\begin{aligned} \left[D^{i}_{B\mathcal{J}_1\mathcal{J}_2}, D^{i}_{B\mathcal{J}_3\mathcal{J}_4}\right] &= \delta_{ij}\left[D^{i}_{B\mathcal{J}_1\mathcal{J}_4}\delta_{\mathcal{J}_2\mathcal{J}_3} - D^{i}_{B\mathcal{J}_3\mathcal{J}_2}\delta_{\mathcal{J}_1\mathcal{J}_4}\right] , \\ \left[D^{i}_{B\mathcal{J}_1\mathcal{J}_2}, \Sigma_{Bj}\right] &= 0 , \\ \left[\Sigma^{(+)}_{Bi}, \Sigma_{Bj}\right] &= 0 , \qquad (i\neq j) , \\ \{\Sigma_{Bi},\Sigma_{Bi}\} &= 0 , \end{aligned} \tag{5.20}$$

Thus the operators $D^{i}_{B\mathcal{J}_1\mathcal{J}_2}$ satisfy the same relations as the operators $D^{i}_{\mathcal{J}_1\mathcal{J}_2}$, given by (4.31), i.e. the results of section 4 can be used directly as far as the interaction terms in $H_{\rm eff}$ are concerned. Next we rewrite the remaining terms using (5.19). Then the following expression is obtained for $H_{\rm eff}$:

$$H_{\rm eff} \;=\; E_{Cl} - \frac{\hbar^2}{8m\alpha}\sum_{i,\hat{\boldsymbol{\xi}}} P^{i}_{B\hat{\boldsymbol{\xi}}} P^{i}_{B\hat{\boldsymbol{\xi}}} + \frac{1}{2}\,\alpha\sum_{i,j}\sum_{\hat{\boldsymbol{\xi}},\hat{\boldsymbol{\eta}}} M_{\hat{\boldsymbol{\xi}}\hat{\boldsymbol{\eta}}}(\boldsymbol{R}_{ij}) S^{i}_{B\hat{\boldsymbol{\xi}}} S^{j}_{B\hat{\boldsymbol{\xi}}} + \sum_{M=3}^{\infty} V^{B}_{M}$$

$$+ \quad i\mu_B B \sum_i \left[S^i_{B\hat{\boldsymbol{x}}} P^i_{B\hat{\boldsymbol{y}}} - S^i_{B\hat{\boldsymbol{y}}} P^i_{B\hat{\boldsymbol{x}}} \right] + \mu_B^2 B^2 \frac{m\alpha}{\hbar^2} \sum_i \sum_{\hat{\boldsymbol{\xi}}=\{\hat{\boldsymbol{x}},\hat{\boldsymbol{y}}\}} S^i_{B\hat{\boldsymbol{\xi}}} S^i_{B\hat{\boldsymbol{\xi}}}$$

$$- \quad \mu_B B \left[2N - \sum_i 2\Sigma^+_{B_i} \Sigma_{B_i} \right] , \tag{5.21}$$

where

$$V_M^B = \frac{1}{2} \sum_{i \neq j} \sum_{\boldsymbol{q}}{}' e^{i\boldsymbol{q}\cdot\boldsymbol{R}_{ij}} \frac{4\pi e^2}{\Omega q^2} e^{-\alpha q^2} \frac{1}{M!} \alpha^{\frac{1}{2}M} \left[i \sum_{\hat{\boldsymbol{\xi}}} (\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}}) (S^i_{B\hat{\boldsymbol{\xi}}} - S^j_{B\hat{\boldsymbol{\xi}}}) \right]^M \tag{5.22}$$

and

$$\begin{aligned} S^i_{B\hat{\boldsymbol{\xi}}} &= \sum_{\boldsymbol{J}} \sqrt{\boldsymbol{J}\cdot\hat{\boldsymbol{\xi}}+1} \left[D^i_{B\boldsymbol{J}+\hat{\boldsymbol{\xi}},\boldsymbol{J}} + D^i_{B\boldsymbol{J},\boldsymbol{J}+\hat{\boldsymbol{\xi}}} \right] , \\ P^i_{B\hat{\boldsymbol{\xi}}} &= \sum_{\boldsymbol{J}} \sqrt{\boldsymbol{J}\cdot\hat{\boldsymbol{\xi}}+1} \left[D^i_{B\boldsymbol{J},\boldsymbol{J}+\hat{\boldsymbol{\xi}}} - D^i_{B\boldsymbol{J}+\hat{\boldsymbol{\xi}},\boldsymbol{J}} \right] . \end{aligned} \tag{5.23}$$

The second rank tensor $\boldsymbol{M}(\boldsymbol{R}_{ij})$ is given by (4.45).

In order to obtain the eigenvalues and eigenstates of the low-density electron system in a homogeneous magnetic field up to order $r_s^{-3/2}$ all higher order terms represented by V_M^B in (5.21) are neglected and the following tensor is introduced:

$$\boldsymbol{M}_B(\boldsymbol{R}_{ij}) = \boldsymbol{M}(\boldsymbol{R}_{ij}) , \qquad i \neq j ,$$

$$\begin{aligned} M_{B\hat{\boldsymbol{\xi}}\hat{\boldsymbol{\eta}}}(0) &= M_{\hat{\boldsymbol{\xi}}\hat{\boldsymbol{\eta}}}(0) + \frac{m\mu_B^2 B^2}{\hbar^2} \left[\delta_{\hat{\boldsymbol{\xi}}\hat{\boldsymbol{x}}} \delta_{\hat{\boldsymbol{\eta}}\hat{\boldsymbol{x}}} + \delta_{\hat{\boldsymbol{\xi}}\hat{\boldsymbol{y}}} \delta_{\hat{\boldsymbol{\eta}}\hat{\boldsymbol{y}}} \right] \\ &= \left(\frac{8\pi N e^2}{3\Omega} + \frac{m\mu_B^2 B^2}{\hbar^2} \left[\delta_{\hat{\boldsymbol{\xi}}\hat{\boldsymbol{x}}} + \delta_{\hat{\boldsymbol{\xi}}\hat{\boldsymbol{y}}} \right] \right) \delta_{\hat{\boldsymbol{\xi}}\hat{\boldsymbol{\eta}}} . \end{aligned} \tag{5.24}$$

In terms of the boson operators

$$\begin{aligned} A_{B\boldsymbol{k}\lambda} &= \frac{1}{\sqrt{2N}} \sum_{i,\hat{\boldsymbol{\xi}}} \left[e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_i} \boldsymbol{\varepsilon}^B_{-\boldsymbol{k}\lambda} \cdot \hat{\boldsymbol{\xi}} \left(\sqrt{\frac{m\omega_{B\boldsymbol{k}\lambda}\alpha}{2\hbar}} S^i_{B\hat{\boldsymbol{\xi}}} + \sqrt{\frac{\hbar}{8m\omega_{B\boldsymbol{k}\lambda}\alpha}} P^i_{B\hat{\boldsymbol{\xi}}} \right) \right] , \\ A^+_{B\boldsymbol{k}\lambda} &= \frac{1}{\sqrt{2N}} \sum_{i,\hat{\boldsymbol{\xi}}} \left[e^{i\boldsymbol{k}\cdot\boldsymbol{R}_i} \boldsymbol{\varepsilon}^B_{\boldsymbol{k}\lambda} \cdot \hat{\boldsymbol{\xi}} \left(\sqrt{\frac{m\omega_{B\boldsymbol{k}\lambda}\alpha}{2\hbar}} S^i_{B\hat{\boldsymbol{\xi}}} - \sqrt{\frac{\hbar}{8m\omega_{B\boldsymbol{k}\lambda}\alpha}} P^i_{B\hat{\boldsymbol{\xi}}} \right) \right] , \end{aligned} \tag{5.25}$$

where $\omega_{B\boldsymbol{k}\lambda}$ and $\epsilon^{B}_{\boldsymbol{k}\lambda}$ are given by the eigenvalue equation

$$\sum_{\iota} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_{\iota}} M_B(\boldsymbol{R}_{\iota})\epsilon^{B}_{\boldsymbol{k}\lambda} = m\omega^2_{B\boldsymbol{k}\lambda}\,\epsilon^{B}_{\boldsymbol{k}\lambda}\,, \tag{5.26}$$

the effective Hamiltonian can then be expressed as

$$\begin{aligned} H_{\text{eff}} &= E_{Cl} + \sum_{\boldsymbol{k}\lambda}\left[\hbar\omega_{B\boldsymbol{k}\lambda}\left[\frac{1}{2} + A^{+}_{B\boldsymbol{k}\lambda}A_{B\boldsymbol{k}\lambda}\right] + \sum_{\lambda'} i\mu_B\boldsymbol{B}\cdot(\epsilon^{B}_{\boldsymbol{k}\lambda'}\times\epsilon^{B}_{\boldsymbol{k}\lambda})A^{+}_{B\boldsymbol{k}\lambda'}A_{B\boldsymbol{k}\lambda}\right] \\ &- \mu_B B\left[2N - \sum_{\iota} 2\Sigma^{+}_{B\iota}\,\Sigma_{B\iota}\right]\,. \end{aligned} \tag{5.27}$$

This Hamiltonian consists of two different parts. The first part describes a system of non-interacting bosons, where the different polarizations λ are mixed because of the magnetic field. The second part represents a system of uncoupled paulions according to (5.19) and (5.20). Both parts commute with each other as follows from (5.20).

The boson part of Hamiltonian (5.27) is a bilinear form of the boson operators and can therefore be diagonalized by the unitary transformation

$$\begin{aligned} B_{\boldsymbol{k}\mu} &= \sum_{\lambda} u_{\lambda\mu}\,A_{B\boldsymbol{k}\lambda}\,, \\ B^{+}_{\boldsymbol{k}\mu} &= \sum_{\lambda} u^{*}_{\lambda\mu}\,A^{+}_{B\boldsymbol{k}\lambda}\,, \end{aligned} \tag{5.28}$$

where

$$\sum_{\lambda} u_{\lambda\mu}\,u^{*}_{\lambda\mu'} = \delta_{\mu\mu'} \tag{5.29}$$

and

$$\sum_{\mu} u_{\lambda\mu}\,u^{*}_{\lambda'\mu} = \delta_{\lambda\lambda'}\,. \tag{5.30}$$

Substituting into (5.27) the inverse transformation

$$\begin{aligned} A_{B\boldsymbol{k}\lambda} &= \sum_{\mu} u^{*}_{\lambda\mu}\,B_{\boldsymbol{k}\mu}\,, \\ A^{+}_{B\boldsymbol{k}\lambda} &= \sum_{\mu} u_{\lambda\mu}\,B^{+}_{\boldsymbol{k}\mu}\,, \end{aligned} \tag{5.31}$$

the effective Hamiltonian can be represented as

$$H_{\text{eff}} = E_{Cl} + \frac{1}{2}\sum_{\boldsymbol{k}\lambda}\hbar\omega_{B\boldsymbol{k}\lambda} + \sum_{\boldsymbol{k}\mu}\hbar E_{\boldsymbol{k}\mu}\,B^{+}_{\boldsymbol{k}\mu}B_{\boldsymbol{k}\mu} - \mu_B B[2N - 2\sum_{\iota}\Sigma^{+}_{B\iota}\,\Sigma_{B\iota}]\,. \tag{5.32}$$

The appearing frequencies $E_{\boldsymbol{k}\mu}$ and the operators $B^{(+)}_{\boldsymbol{k}\mu}$ are determined by the eigenvalue equation

$$\sum_{\lambda'} \Omega^{\boldsymbol{k}}_{\lambda\lambda'} u_{\lambda'\mu} = E_{\boldsymbol{k}\mu} u_{\lambda\mu} \ , \tag{5.33}$$

where the hermitean matrix $\Omega^{\boldsymbol{k}}$ is given by

$$\Omega^{\boldsymbol{k}}_{\lambda\lambda'} = \omega_{B\boldsymbol{k}\lambda}\delta_{\lambda\lambda'} + i\frac{\mu_B \boldsymbol{B}}{\hbar} \cdot (\boldsymbol{\varepsilon}^{B}_{\boldsymbol{k}\lambda'} \times \boldsymbol{\varepsilon}^{B}_{\boldsymbol{k}\lambda}) \ . \tag{5.34}$$

The eigenvalues $E_{\boldsymbol{k}\mu}$ are the solutions of the following third order algebraic equation:

$$\begin{aligned}(E_{\boldsymbol{k}\mu} - \omega_{B\boldsymbol{k}1})(E_{\boldsymbol{k}\mu} - \omega_{B\boldsymbol{k}2})(E_{\boldsymbol{k}\mu} - \omega_{B\boldsymbol{k}3}) = \\ \omega^2_{c23}(E_{\boldsymbol{k}\mu} - \omega_{B\boldsymbol{k}1}) + \omega^2_{c31}(E_{\boldsymbol{k}\mu} - \omega_{B\boldsymbol{k}2}) + \omega^2_{c12}(E_{\boldsymbol{k}\mu} - \omega_{B\boldsymbol{k}3}) \ ,\end{aligned} \tag{5.35}$$

with

$$\omega_{c\lambda\lambda'} = \frac{\mu_B \boldsymbol{B}}{\hbar} \cdot (\boldsymbol{\varepsilon}^{B}_{\boldsymbol{k}\lambda'} \times \boldsymbol{\varepsilon}^{B}_{\boldsymbol{k}\lambda}) \ . \tag{5.36}$$

Thus the energy spectrum of the original Hamiltonian (5.1) is known up to order $r_s^{-3/2}$, as follows from the expression (5.32) which is the sum of a free boson and an uncoupled paulion system. The corresponding eigenstates are given by

$$|\psi^B_n\rangle = \prod_{\boldsymbol{k},\mu} \frac{1}{\sqrt{n_{\boldsymbol{k}\mu}!}} \left(B^{+}_{\boldsymbol{k}\mu}\right)^{n_{\boldsymbol{k}\mu}} \prod_{i} (\Sigma^{+}_{Bi})^{n_i} |\psi^B_0\rangle \ , \tag{5.37}$$

where $n_{\boldsymbol{k}\mu}$ and n_i are boson and fermion occupation numbers, respectively, i.e. $n_{\boldsymbol{k}\mu} = 0, 1, 2, 3, \ldots$ and $n_i = 0, 1$. The ground state $|\psi^B_0\rangle$ is obtained using the representation (5.3) and

$$\Sigma_{Bi}|\psi^B_0\rangle = B_{\boldsymbol{k}\mu}|\psi^B_0\rangle = 0 \tag{5.38}$$

for all i, $\boldsymbol{k}$ and μ. As expected all spins are directed along the magnetic field in the ground state.

The thermodynamic properties at low temperatures $T = \frac{1}{k_B\beta}$ follow directly from the internal energy

$$E = E_{Cl} + \frac{1}{2}\sum_{\boldsymbol{k}\lambda} \hbar\omega_{B\boldsymbol{k}\lambda} - 2N\mu_B B + \sum_{\boldsymbol{k}\mu} \hbar E_{\boldsymbol{k}\mu}[e^{\beta\hbar E_{\boldsymbol{k}\mu}} - 1]^{-1} + 4N\mu_B B[e^{2\mu_B B\beta} + 1]^{-1} \ . \tag{5.39}$$

Finally we have to show that a homogeneous field in the jellium model can exist according to Maxwell's equations. This means that the response of the system to the supposed homogeneous field, i.e. the current density, must be calculated. The current density operator $\boldsymbol{\jmath}(\boldsymbol{r})$, which is defined by the equation of continuity, is for the present system

$$\boldsymbol{\jmath}(\boldsymbol{r}) = \sum_{\sigma} \left[-\frac{i e\hbar}{2m} [\psi_\sigma^+(\boldsymbol{r}) \boldsymbol{\nabla} \psi_\sigma(\boldsymbol{r}) - (\boldsymbol{\nabla}\psi_\sigma^+(\boldsymbol{r}))\psi_\sigma(\boldsymbol{r})] - \frac{e^2}{mc} \boldsymbol{A}(\boldsymbol{r}) \psi_\sigma^+(\boldsymbol{r}) \psi_\sigma(\boldsymbol{r}) \right] , \quad (5.40)$$

where $\boldsymbol{A}(\boldsymbol{r})$ is given by (5.2). Analogous to the Hamilton operator the current density operator can be replaced as well by an effective operator having the same eigenvalue spectrum as $\boldsymbol{\jmath}(\boldsymbol{r})$ provided that overlap is neglected. This effective current density operator is given by

$$\boldsymbol{\jmath}_{\text{eff}}(\boldsymbol{r}) = \sum_{\boldsymbol{\imath}} \sum_{\boldsymbol{\jmath}_1 \boldsymbol{\jmath}_2} \boldsymbol{\jmath}'_{\boldsymbol{\jmath}_1 \boldsymbol{\jmath}_2}(\boldsymbol{r})\, D'_{B\boldsymbol{\jmath}_1 \boldsymbol{\jmath}_2} , \quad (5.41)$$

where

$$\begin{aligned} \boldsymbol{\jmath}'_{\boldsymbol{\jmath}_1 \boldsymbol{\jmath}_2}(\boldsymbol{r}) &= -\frac{i e\hbar}{2m} \left[f^{*B}_{\boldsymbol{\jmath}_1 \boldsymbol{R}_\imath}(\boldsymbol{r} - \boldsymbol{R}_\imath) \boldsymbol{\nabla} f^{B}_{\boldsymbol{\jmath}_2 \boldsymbol{R}_\imath}(\boldsymbol{r} - \boldsymbol{R}_\imath) - f^{B}_{\boldsymbol{\jmath}_2 \boldsymbol{R}_\imath}(\boldsymbol{r} - \boldsymbol{R}_\imath) \boldsymbol{\nabla} f^{*B}_{\boldsymbol{\jmath}_1 \boldsymbol{R}_\imath}(\boldsymbol{r} - \boldsymbol{R}_\imath) \right] \\ &- \frac{e^2}{mc} \boldsymbol{A}(\boldsymbol{r}) f^{*B}_{\boldsymbol{\jmath}_1 \boldsymbol{R}_\imath}(\boldsymbol{r} - \boldsymbol{R}_\imath) f^{B}_{\boldsymbol{\jmath}_2 \boldsymbol{R}_\imath}(\boldsymbol{r} - \boldsymbol{R}_\imath) . \end{aligned} \quad (5.42)$$

Substituting (5.9) into (5.42) we obtain

$$\begin{aligned} \boldsymbol{\jmath}'_{\boldsymbol{\jmath}_1 \boldsymbol{\jmath}_2}(\boldsymbol{r}) &= \frac{-i e\hbar}{2m} \left[f^*_{\boldsymbol{\jmath}_1}(\boldsymbol{r} - \boldsymbol{R}_\imath) \boldsymbol{\nabla} f_{\boldsymbol{\jmath}_2}(\boldsymbol{r} - \boldsymbol{R}_\imath) - f_{\boldsymbol{\jmath}_2}(\boldsymbol{r} - \boldsymbol{R}_\imath) \boldsymbol{\nabla} f^*_{\boldsymbol{\jmath}_1}(\boldsymbol{r} - \boldsymbol{R}_\imath) \right] \\ &- \frac{e^2}{mc} [\boldsymbol{A}(\boldsymbol{r}) - \boldsymbol{A}(\boldsymbol{R}_\imath)] f^*_{\boldsymbol{\jmath}_1}(\boldsymbol{r} - \boldsymbol{R}_\imath) f_{\boldsymbol{\jmath}_2}(\boldsymbol{r} - \boldsymbol{R}_\imath) . \end{aligned} \quad (5.43)$$

It should be remarked that the current density operator as given by (5.41) and (5.43) can be interpreted in terms of electrons moving around lattice sites. Hopping does not appear because overlap is neglected.

The full translational symmetry of the original Hamiltonian (5.1) implies that the current density $\boldsymbol{\jmath}$ must be homogeneous as well. That quantity is obtained in the usual way by averaging the symmetry-broken thermal average $\langle \boldsymbol{\jmath}_{\text{eff}}(\boldsymbol{r}) \rangle$ over a unit cell of the Wigner lattice, i.e.

$$\boldsymbol{\jmath} = \frac{1}{\Omega_{\text{cell}}} \int_{\text{unit cell}} d^3 r \langle \boldsymbol{\jmath}_{\text{eff}}(\boldsymbol{r} + \boldsymbol{R}_\imath) \rangle , \quad (5.44)$$

where $\Omega_{\rm cell}$ and $\boldsymbol{R}_i$ denote the volume and position of the unit cell, respectively. Substituting (5.41) into (5.44) and neglecting all terms containing $\exp[-R_{ij}^2/2\alpha]$, $i \neq j$, as they are of the order of the overlap, we obtain

$$\boldsymbol{\jmath} = \frac{1}{\Omega_{\rm cell}} \int_{\rm all\ space} d^3r \sum_{\mathcal{J}_1\mathcal{J}_2} \jmath'_{\mathcal{J}_1\mathcal{J}_2}(\boldsymbol{r}+\boldsymbol{R}_i)\langle D'_{\mathcal{J}_1\mathcal{J}_2}\rangle \ , \tag{5.45}$$

where $\jmath'_{\mathcal{J}_1\mathcal{J}_2}$ is given by (5.43). Because $\langle D'_{\mathcal{J}_1\mathcal{J}_2}\rangle$ is invariant under lattice translations the uniform current density can now be expressed as

$$\begin{aligned}
\boldsymbol{\jmath} &= \frac{1}{2N}\sum_i \frac{1}{\Omega_{\rm cell}} \int d^3r \sum_{\mathcal{J}_1\mathcal{J}_2} \jmath'_{\mathcal{J}_1\mathcal{J}_2}(\boldsymbol{r})\langle D'_{\mathcal{J}_1\mathcal{J}_2}\rangle = \frac{1}{\Omega}\int d^3r \langle \jmath_{\rm eff}(\boldsymbol{r})\rangle \\
&= \frac{-ieh}{2m\sqrt{\alpha}\,\Omega}\sum_{i,\hat{\boldsymbol{\xi}}}\langle P'_{i\hat{\boldsymbol{\xi}}}\rangle\hat{\boldsymbol{\xi}} - \frac{e^2B\sqrt{\alpha}}{2mc\Omega}\sum_i\left[\langle S'_{iB\hat{\boldsymbol{x}}}\rangle\hat{\boldsymbol{y}} - \langle S'_{iB\hat{\boldsymbol{y}}}\rangle\hat{\boldsymbol{x}}\right] \ ,
\end{aligned} \tag{5.46}$$

where $S'_{iB\hat{\boldsymbol{\xi}}}$ and $P'_{iB\hat{\boldsymbol{\xi}}}$ are given by (5.23). From (5.25) and (5.31) we get

$$\begin{aligned}
S'_{iB\hat{\boldsymbol{\xi}}} &= \frac{1}{\sqrt{2N}}\sum_{\boldsymbol{k},\lambda,\mu} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_i}\,\epsilon_{\boldsymbol{k}\lambda}\cdot\hat{\boldsymbol{\xi}}\sqrt{\frac{\hbar}{2m\omega_{B\boldsymbol{k}\lambda^\alpha}}}\,[u_{\lambda\mu}B^+_{\boldsymbol{k}\mu} + u^*_{\lambda\mu}B_{-\boldsymbol{k}\mu}] \ , \\
P'_{iB\hat{\boldsymbol{\xi}}} &= \frac{1}{\sqrt{2N}}\sum_{\boldsymbol{k},\lambda,\mu} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_i}\,\epsilon_{\boldsymbol{k}\lambda}\cdot\hat{\boldsymbol{\xi}}\sqrt{\frac{2m\omega_{B\boldsymbol{k}\lambda^\alpha}}{\hbar}}\,[u^*_{\lambda\mu}B_{\boldsymbol{k}\mu} - u_{\lambda\mu}B^+_{-\boldsymbol{k}\mu}] \ .
\end{aligned} \tag{5.47}$$

Substituting (5.47) into (5.46) and using that for $\boldsymbol{k}=0$ the solutions of the eigenvalue equation (5.26) are given by $m\omega^2_{B01} = m\omega^2_{B02} = \frac{8\pi Ne^2}{3\Omega} + \frac{\mu_B^2B^2m}{\hbar^2}$, $m\omega^2_{B03} = \frac{8\pi Ne^2}{3\Omega}$ and $\boldsymbol{\epsilon}_{01} = \hat{\boldsymbol{x}}$, $\boldsymbol{\epsilon}_{02} = \hat{\boldsymbol{y}}$, $\boldsymbol{\epsilon}_{03} = \hat{\boldsymbol{z}}$, we arrive at

$$\begin{aligned}
\boldsymbol{\jmath} &= \frac{\sqrt{2N}}{\Omega}\sum_\mu e\sqrt{\frac{\hbar}{2m}}\left[\left(\frac{8\pi Ne^2}{3m\Omega} + \frac{\mu_B^2B^2}{\hbar^2}\right)^{1/4} 2\,\mathrm{Im}\,(u_{1\mu}\langle B^+_{o\mu}\rangle\hat{\boldsymbol{x}} + u_{2\mu}\langle B^+_{o\mu}\rangle\hat{\boldsymbol{y}})\right. \\
&+ \left(\frac{8\pi Ne^2}{3m\Omega}\right)^{1/4} 2\,\mathrm{Im}\,(u_{3\mu}\langle B^+_{o\mu}\rangle\hat{\boldsymbol{z}}) \\
&- \left.\left(\frac{8\pi Ne^2}{3m\Omega} + \frac{\mu_B^2B^2}{\hbar^2}\right)^{-1/4}\frac{eB}{mc}\,\mathrm{Re}(u_{1\mu}\langle B^+_{o\mu}\rangle\hat{\boldsymbol{y}} - u_{2\mu}\langle B^+_{o\mu}\rangle\hat{\boldsymbol{x}})\right] \ ,
\end{aligned} \tag{5.48}$$

where $\mathrm{Re}(z)$ and $\mathrm{Im}(z)$ denote the real and imaginary part of the complex number z, respectively. Clearly $\langle B^+_{o\mu}\rangle = 0$ in the free boson approximation (5.32), i.e. $\boldsymbol{\jmath} = 0$.

That conclusion also holds for the interacting boson system described by (5.21), as can be seen in the following way. The eigenstates required to calculate $\langle B^+_{0\mu}\rangle$ are now eigenstates of Hamiltonian (5.21). These states, when represented as linear combinations of the eigenstates $|\psi^B_n\rangle$ of the free boson Hamiltonian (5.32), have the property that they do not contain simultaneously the terms $|\psi^B_n\rangle$ and $B^+_{0\mu}|\psi^B_n\rangle$. That property, which immediately implies $\langle B^+_{0\mu}\rangle = 0$, follows directly from the calculation of the matrix elements $\langle\psi^B_n|V^B_M\, B^+_{0\mu}|\psi^B_n\rangle$, which are zero due to the structure of V^B_M given by (5.22) and (5.47).

Now it can be concluded that the low-density jellium model indeed allows a homogeneous internal magnetic field. For $\boldsymbol{j} = 0$ and the Maxwell equations do give such a field.

B. Response to an inhomogeneous magnetic field

Part A deals with a low-density jellium model having a homogeneous internal magnetic field. The question, however, whether an external magnetic field can penetrate into the system thus creating the internal field, is not answered. For an answer to that question requires the introduction of boundaries and external field sources, which destroy the translational invariance explicitly used in part A. The situation that a magnetic field does not penetrate a given system is known as the Meissner-Ochsenfeld effect. In order to discuss the eventual appearance of that effect in the low-density model we calculate, analogous to the procedure of the B.C.S.-theory [17, 18], the response of the system to an inhomogeneous magnetic field. Such a field is generated by some source current density in the interior of the still infinite system.

In order to examine the possible existence of the Meissner-Ochsenfeld effect we only need to calculate the linear response of the system to the magnetic field, i.e. the linear relation between the induced current density $\boldsymbol{j}(\boldsymbol{r},t)$ and the vector potential $\boldsymbol{A}(\boldsymbol{r},t)$. This means that the magnetic field is assumed to be very small and all terms of order $|\boldsymbol{A}|^n$, $n \geq 2$, are neglected.

The criterion for the appearance of the Meissner-Ochsenfeld effect is [18]

$$\lim_{q\to 0}\lim_{\omega\to 0} \boldsymbol{\jmath}(\boldsymbol{q},\omega) = -K \lim_{q\to 0}\lim_{\omega\to 0} \boldsymbol{A}(\boldsymbol{q},\omega) \ , \tag{5.49}$$

where K is a non-zero constant and $\boldsymbol{\jmath}(\boldsymbol{q},\omega)$ and $\boldsymbol{A}(\boldsymbol{q},\omega)$ are given by the Fourier decompositions

$$\begin{aligned} \boldsymbol{A}(\boldsymbol{r},t) &= \frac{1}{\Omega}\sum_{\boldsymbol{q}} \boldsymbol{A}(\boldsymbol{q},t)\, e^{i\boldsymbol{q}\cdot\boldsymbol{r}} = \frac{1}{\Omega}\sum_{\boldsymbol{q}} \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, \boldsymbol{A}(\boldsymbol{q},\omega) e^{i\boldsymbol{q}\cdot\boldsymbol{r}} e^{-i\omega t} \ , \\ \boldsymbol{\jmath}(\boldsymbol{r},t) &= \frac{1}{\Omega}\sum_{\boldsymbol{q}} \boldsymbol{\jmath}(\boldsymbol{q},t)\, e^{i\boldsymbol{q}\cdot\boldsymbol{r}} = \frac{1}{\Omega}\sum_{\boldsymbol{q}} \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, \boldsymbol{\jmath}(\boldsymbol{q},\omega) e^{i\boldsymbol{q}\cdot\boldsymbol{r}} e^{-i\omega t} \ . \end{aligned} \tag{5.50}$$

The condition (5.49) is a relation between macroscopic quantities. This means in the present case that the local field and current density must be averaged over one unit cell of the Wigner lattice. It should be remarked that the resulting macroscopic quantities are no longer identical here to the microscopic ones as contrasted with the situation discussed in part A.

Up to order $|\boldsymbol{A}|$ the Hamiltonian can be expressed as

$$H = H(0) + H(1) + H_s \ , \tag{5.51}$$

where $H(0)$ is the Hamiltonian (3.1) of the jellium model, H_s is the term describing the interaction between the electron spins and the magnetic field, and $H(1)$ is given by

$$H(1) = \frac{-\mu_B}{\Omega}\sum_{\boldsymbol{k},\boldsymbol{q}}\sum_{\sigma} (2\boldsymbol{k}+\boldsymbol{q})\cdot\boldsymbol{A}(\boldsymbol{q},t)\, c^{+}_{\boldsymbol{k}+\boldsymbol{q}\sigma} c_{\boldsymbol{k}\sigma} \ . \tag{5.52}$$

The explicit form of H_s is not given here, as H_s does not affect the current density for the following two reasons. First of all H_s commutes with the charge density operator $\rho(\boldsymbol{r}) = \sum_{\sigma} \psi^{+}_{\sigma}(\boldsymbol{r})\psi_{\sigma}(\boldsymbol{r})$, i.e. H_s plays no part in the equation of continuity that determines the current density operator. Secondly the neglect of the overlap between one-electron wave functions localized at different lattice sites entails that the only effect of H_s on the eigenstates of $H(0)+H(1)$ is the removal of the degeneracy of these states with respect to all possible spin configurations of the lattice. Clearly then we only need to consider the Hamiltonian $\widetilde{H} = H(0) + H(1)$.

Next we replace $H(1)$ by an effective Hamiltonian $H(1)_{\rm eff}$ analogous to the procedure discussed in section 4, i.e. we neglect the effect of exchange:

$$H(1)_{\rm eff} = \frac{-\mu_B}{\Omega} \sum_{\boldsymbol{q},i} \sum_{\boldsymbol{\jmath}_1\boldsymbol{\jmath}_2} e^{i\boldsymbol{q}\cdot\boldsymbol{R}_i} \boldsymbol{A}(\boldsymbol{q},t)\cdot\left[\int d^3k(2\boldsymbol{k}+\boldsymbol{q})\ \hat{f}^*_{\boldsymbol{\jmath}_1}(\boldsymbol{k}+\boldsymbol{q})\hat{f}_{\boldsymbol{\jmath}_2}(\boldsymbol{k})\right] D^{\rm i}_{\boldsymbol{\jmath}_1\boldsymbol{\jmath}_2}\ , \tag{5.53}$$

where $\hat{f}_{\boldsymbol{\jmath}}$ and $D^{\rm i}_{\boldsymbol{\jmath}_1\boldsymbol{\jmath}_2}$ are given by (4.15) and (4.31), respectively. The boson representation of this Hamiltonian is obtained in the following way. Using the relation for the Hermite polynomials,

$$(\boldsymbol{k}\cdot\hat{\boldsymbol{\xi}})H_{\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}}(\boldsymbol{k}\cdot\hat{\boldsymbol{\xi}}\sqrt{2\alpha}) = \frac{1}{\sqrt{2\alpha}}\left[\frac{1}{2}H_{\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}+1}(\boldsymbol{k}\cdot\hat{\boldsymbol{\xi}}\sqrt{2\alpha}) + (\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}})H_{\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}-1}(\boldsymbol{k}\cdot\hat{\boldsymbol{\xi}}\sqrt{2\alpha})\right]\ , \tag{5.54}$$

we arrive at

$$\begin{aligned}
&\sum_{\boldsymbol{\jmath}_1\boldsymbol{\jmath}_2}\left[\int d^3k(2\boldsymbol{k}+\boldsymbol{q})\,\hat{f}^*_{\boldsymbol{\jmath}_1}(\boldsymbol{k}+\boldsymbol{q})\hat{f}_{\boldsymbol{\jmath}_2}(\boldsymbol{k})\right] D^{\rm i}_{\boldsymbol{\jmath}_1\boldsymbol{\jmath}_2} = \\
&\quad\sum_{\boldsymbol{\jmath}_1\boldsymbol{\jmath}_2,\hat{\boldsymbol{\xi}}} \frac{i\hat{\boldsymbol{\xi}}}{2\sqrt{\alpha}}\left[\int d^3k\hat{f}^*_{\boldsymbol{\jmath}_1}(\boldsymbol{k}+\boldsymbol{q})\hat{f}_{\boldsymbol{\jmath}_2}(\boldsymbol{k})\right]\left[\sqrt{\boldsymbol{\jmath}_1\cdot\hat{\boldsymbol{\xi}}+1}\,(D^{\rm i}_{\boldsymbol{\jmath}_1+\hat{\boldsymbol{\xi}},\boldsymbol{\jmath}_2} - D^{\rm i}_{\boldsymbol{\jmath}_2,\boldsymbol{\jmath}_1+\hat{\boldsymbol{\xi}}})\right. \\
&\quad\left.+\sqrt{\boldsymbol{\jmath}_1\cdot\hat{\boldsymbol{\xi}}}\,(D^{\rm i}_{\boldsymbol{\jmath}_2,\boldsymbol{\jmath}_1-\hat{\boldsymbol{\xi}}} - D^{i}_{\boldsymbol{\jmath}_1-\hat{\boldsymbol{\xi}},\boldsymbol{\jmath}_2})\right] \qquad = \\
&\quad-\sum_{\boldsymbol{\jmath}_1\boldsymbol{\jmath}_2,\hat{\boldsymbol{\xi}}} \frac{i\hat{\boldsymbol{\xi}}}{2\sqrt{\alpha}}\left[\int d^3k\hat{f}^*_{\boldsymbol{\jmath}_1}(\boldsymbol{k}+\boldsymbol{q})\hat{f}_{\boldsymbol{\jmath}_2}(\boldsymbol{k})\right]\left[D^{\rm i}_{\boldsymbol{\jmath}_2\boldsymbol{\jmath}_1}P^{\rm i}_{\hat{\boldsymbol{\xi}}} + P^{\rm i}_{\hat{\boldsymbol{\xi}}}D^{\rm i}_{\boldsymbol{\jmath}_1\boldsymbol{\jmath}_2}\right]\ ,
\end{aligned} \tag{5.55}$$

where $P^{\rm i}_{\hat{\boldsymbol{\xi}}}$ is given by (4.47) and use is made of (4.35). Next we expand the right hand side of (5.55) in terms of the components of $\sqrt{\alpha}\ \boldsymbol{q}$. Such an expansion is explicitly done up to fourth order in Appendix V. The resulting expression (V.5) can be directly generalized to the following result:

$$\begin{aligned}
&\sum_{\boldsymbol{\jmath}_1\boldsymbol{\jmath}_2}\left[\int d^3k\,\hat{f}^*_{\boldsymbol{\jmath}_1}(\boldsymbol{k}+\boldsymbol{q})\hat{f}_{\boldsymbol{\jmath}_2}(\boldsymbol{k})\right] D^{\rm i}_{\boldsymbol{\jmath}_1\boldsymbol{\jmath}_2} = \\
&\qquad 1+\chi_0(\boldsymbol{q}) + \sum_{M=1}^{\infty}\sum_{\hat{\boldsymbol{\xi}}_1\cdots\hat{\boldsymbol{\xi}}_M}\chi_{\hat{\boldsymbol{\xi}}_1\cdots\hat{\boldsymbol{\xi}}_M}(\boldsymbol{q})\,S^{\rm i}_{\hat{\boldsymbol{\xi}}_1}S^{\rm i}_{\hat{\boldsymbol{\xi}}_2}\cdots S^{\rm i}_{\hat{\boldsymbol{\xi}}_M}\ ,
\end{aligned} \tag{5.56}$$

where $S^{\rm i}_{\hat{\boldsymbol{\xi}}}$ is given by (4.40) and the functions χ_0 and $\chi_{\hat{\boldsymbol{\xi}}_1\cdots\hat{\boldsymbol{\xi}}_M}$ satisfy

$$\lim_{\boldsymbol{q}\to 0}\chi_0(\boldsymbol{q}) = \lim_{\boldsymbol{q}\to 0}\chi_{\hat{\boldsymbol{\xi}}_1\cdots\hat{\boldsymbol{\xi}}_M}(\boldsymbol{q}) = 0\ . \tag{5.57}$$

Substitution of (5.55) and (5.56) into (5.53) gives

$$H(1)_{\rm eff} = \frac{\mu_B i}{\Omega\sqrt{\alpha}} \sum_{\boldsymbol{q},i,\hat{\boldsymbol{\xi}}} \boldsymbol{A}(\boldsymbol{q},t)\cdot\hat{\boldsymbol{\xi}}\, e^{i\boldsymbol{q}\cdot\boldsymbol{R}_i}\left[P^i_{\hat{\boldsymbol{\xi}}}[1+\chi_0(\boldsymbol{q})]\right.$$
$$\left. + \sum_{M=1}^{\infty}\sum_{\hat{\boldsymbol{\xi}}_1\cdots\hat{\boldsymbol{\xi}}_M} \frac{1}{2}\chi_{\hat{\boldsymbol{\xi}}_1\cdots\hat{\boldsymbol{\xi}}_M}(\boldsymbol{q})\left[P^i_{\hat{\boldsymbol{\xi}}}S^i_{\hat{\boldsymbol{\xi}}_1}\cdots S^i_{\hat{\boldsymbol{\xi}}_M} + S^i_{\hat{\boldsymbol{\xi}}_1}\cdots S^i_{\hat{\boldsymbol{\xi}}_M}P^i_{\hat{\boldsymbol{\xi}}}\right]\right]. \quad (5.58)$$

This Hamiltonian can be easily expressed in terms of the boson operators $A^{(+)}_{\boldsymbol{k}\lambda}$, using (4.51) and (4.54).

The relevant Hamiltonian, $\widetilde{H} = H(0) + H(1)$, can now be replaced by the following effective Hamiltonian:

$$\widetilde{H}_{\rm eff} = H(0)_{\rm eff} + H(1)_{\rm eff}\ , \quad (5.59)$$

where, as shown in Appendix V, $H(0)_{\rm eff}$ has the following form

$$H(0)_{\rm eff} = E_{Cl} + \sum_{\boldsymbol{k}\lambda}[\frac{1}{2} + A^+_{\boldsymbol{k}\lambda}A_{\boldsymbol{k}\lambda}]\hbar\omega_{\boldsymbol{k}\lambda} + \sum_{M=3}^{\infty} V_M\ , \quad (5.60)$$

with

$$V_M = N\sum_{\boldsymbol{K}_n}\sum_{\boldsymbol{R}_i\neq 0}\sum_{\boldsymbol{q}_0}{}' e^{i\boldsymbol{q}_0\boldsymbol{R}_i}\frac{4\pi e^2}{\Omega q_0^2}e^{-\alpha q_0^2}\frac{i^M}{M!}\sum_{\substack{\boldsymbol{k}_1\ldots\boldsymbol{k}_M\\ \lambda_1\ldots\lambda_M}}\delta_{\boldsymbol{k}_1+\ldots+\boldsymbol{k}_M,\boldsymbol{K}_n}\prod_{j=1}^{M}$$
$$\left[\sqrt{\frac{\hbar}{4Nm\omega_{\boldsymbol{k}_j\cdot\lambda_j}}}\boldsymbol{\varepsilon}_{\boldsymbol{k}_j\lambda_j}\cdot\boldsymbol{q}_0[e^{-i\boldsymbol{k}_j\cdot\boldsymbol{R}_i}-1][A^+_{\boldsymbol{k}_j\lambda_j} + A_{-\boldsymbol{k}_j\lambda_j}]\right]\ , \quad (5.61)$$

whereas $H(1)_{\rm eff}$ is given by

$$H(1)_{\rm eff} = \frac{\mu_B i\sqrt{2N}}{\Omega}\sum_{\boldsymbol{K}_n}\sum_{\boldsymbol{k}\lambda}\sqrt{\frac{2m\omega_{\boldsymbol{k}\lambda}}{\hbar}}\left\{\boldsymbol{A}(\boldsymbol{k}+\boldsymbol{K}_n,t)\cdot\boldsymbol{\varepsilon}_{\boldsymbol{k}\lambda}\right.$$
$$\times\ [1+\chi_0(\boldsymbol{k}+\boldsymbol{K}_n)][A_{\boldsymbol{k}\lambda} - A^+_{-\boldsymbol{k}\lambda}]$$
$$+\ \frac{1}{2}\sum_{M=1}^{\infty}\sum_{\hat{\boldsymbol{\xi}}_1\cdots\hat{\boldsymbol{\xi}}_M}\sum_{\boldsymbol{k}_1\ldots\boldsymbol{k}_M,\lambda_1\ldots\lambda_M}\boldsymbol{A}(\boldsymbol{k}+\boldsymbol{K}_n-(\boldsymbol{k}_1+\ldots+\boldsymbol{k}_M),t)\cdot\boldsymbol{\varepsilon}_{\boldsymbol{k}\lambda}$$

$$\times \quad [\chi_{\hat{\boldsymbol{\xi}}_1 \cdot \hat{\boldsymbol{\xi}}_M}(\boldsymbol{k} + \boldsymbol{K}_n - (\boldsymbol{k}_1 + \ldots + \boldsymbol{k}_M))]$$

$$\times \quad \left[\left(\prod_{j=1}^{M} \sqrt{\frac{\hbar}{4Nm\alpha\omega_{\boldsymbol{k}_j\lambda_j}}}\, \boldsymbol{\epsilon}_{\boldsymbol{k}_j\lambda_j} \cdot \hat{\boldsymbol{\xi}}_j [A^{\dagger}_{\boldsymbol{k}_j\lambda_j} + A_{-\boldsymbol{k}_j\lambda_j}]\right) [A_{\boldsymbol{k}\lambda} - A^{+}_{-\boldsymbol{k}\lambda}]\right.$$

$$\left. + \quad [A_{\boldsymbol{k}\lambda} - A^{\dagger}_{\boldsymbol{k}\lambda}] \left(\prod_{j=1}^{M} \sqrt{\frac{\hbar}{4Nm\alpha\omega_{\boldsymbol{k}_j\lambda_j}}}\, \boldsymbol{\epsilon}_{\boldsymbol{k}_j\lambda_j} \cdot \hat{\boldsymbol{\xi}}_j [A^{\dagger}_{\boldsymbol{k}_j\lambda_j} + A_{-\boldsymbol{k}_j\lambda_j}]\right)\right]\Bigg\} \cdot \tag{5.62}$$

The summation over $\boldsymbol{K}_n$ in (5.61) and (5.62) runs over all reciprocal lattice vectors. In obtaining (5.61) and (5.62) we assumed that the origin of our coordinate system coincides with a site of the Wigner lattice. That assumption does not influence our conclusion concerning the eventual appearance of the Meissner-Ochsenfeld effect as we are only interested in the macroscopic current density.

Now we discuss an important property of the eigenstates $|\varphi_n\rangle$ of $H(0)_{\text{eff}}$ for the sake of the calculation of the current density. The states $|\varphi_n\rangle$ are linear combinations of the eigenstates $|\psi_m\rangle$ of the free boson term of (5.60). For convenience' sake this complete set of states $|\psi_m\rangle$ is divided into subsets consisting of those eigenstates $|\psi_{l\boldsymbol{K}}\rangle$ that have the same total wave vector $\boldsymbol{K}$ given by

$$\boldsymbol{K} = \sum_{\boldsymbol{k}\lambda} n_{\boldsymbol{k}\lambda}\boldsymbol{k} \tag{5.63}$$

with $n_{\boldsymbol{k}\lambda} = 0, 1, 2, \ldots$ being the occupation number of the one-boson state $|\boldsymbol{k}\lambda\rangle$. Because of the factor $\delta_{\boldsymbol{k}_1+\ldots+\boldsymbol{k}_M,\boldsymbol{K}_n}$ in (5.61) the complete set of eigenstates $|\varphi_n\rangle$ of $H(0)_{\text{eff}}$ can now be divided into subsets consisting of eigenstates $|\varphi_{n\boldsymbol{K}}\rangle$ satisfying

$$|\varphi_{n\boldsymbol{K}}\rangle = \sum_{\boldsymbol{K}_n} \sum_{l} C^{n}_{l\boldsymbol{K}_n} |\psi_{l\boldsymbol{K}+\boldsymbol{K}_n}\rangle \ , \tag{5.64}$$

where the summation over l runs over the subset consisting of states that have the total wave vector $\boldsymbol{K} + \boldsymbol{K}_n$ and the constants $C^{n}_{l\boldsymbol{K}_n}$ satisfy

$$\sum_{\boldsymbol{K}_n} \sum_{l} |C^{n}_{l\boldsymbol{K}_n}|^2 = 1 \ . \tag{5.65}$$

Thus the eigenstates $|\varphi_n\rangle$ have the following property:

$$\langle\varphi_n|\prod_j (A^\dagger_{\boldsymbol{k}_j\lambda_j} + \mathrm{sgn}(j) A_{-\boldsymbol{k}_j\lambda_j})|\varphi_n\rangle = 0 \quad \text{for} \quad \sum_j \boldsymbol{k}_j \neq \boldsymbol{K}_n \,, \tag{5.66}$$

where $\mathrm{sgn}(j) = +1$ or $\mathrm{sgn}(j) = -1$ and $\boldsymbol{K}_n$ may be any reciprocal lattice vector.

The current density operator, which follows from the equation of continuity, is given by

$$\boldsymbol{j}(\boldsymbol{r},t) = \frac{1}{\Omega}\sum_{\boldsymbol{q}} [\boldsymbol{j}^P(\boldsymbol{q},t) + \boldsymbol{j}^D(\boldsymbol{q},t)] e^{i\boldsymbol{q}\,\boldsymbol{r}} \,, \tag{5.67}$$

where

$$\boldsymbol{j}^P(\boldsymbol{q},t) = \frac{e\hbar}{2m}\sum_{\boldsymbol{k}\sigma} [2\boldsymbol{k}+\boldsymbol{q}]\, c^+_{\boldsymbol{k}+\boldsymbol{q}\sigma} c_{\boldsymbol{k}\sigma} \tag{5.68}$$

and

$$\boldsymbol{j}^D(\boldsymbol{q},t) = \frac{-e^2}{mc\Omega}\sum_{\boldsymbol{k},\boldsymbol{q}',\sigma} \boldsymbol{A}(\boldsymbol{q}-\boldsymbol{q}',t)\, c_{\boldsymbol{k}+\boldsymbol{q}'\sigma} c_{\boldsymbol{k}\sigma} \tag{5.69}$$

are the Fourier transforms of the paramagnetic and diamagnetic current density operator, respectively. The effective operators corresponding with $\boldsymbol{j}^P(\boldsymbol{q},t)$ and $\boldsymbol{j}^D(\boldsymbol{q},t)$ read

$$\boldsymbol{j}^P_{\mathrm{eff}}(\boldsymbol{q},t) = \frac{e\hbar}{2m}\sum_{\imath}\sum_{\jmath_1\jmath_2} e^{i\boldsymbol{q}\,\boldsymbol{R}_\imath}\Big[\int d^3k (2\boldsymbol{k}+\boldsymbol{q}) \hat{f}^*_{\jmath_1}(\boldsymbol{k}+\boldsymbol{q}) \hat{f}_{\jmath_2}(\boldsymbol{k})\Big] D^\imath_{\jmath_1\jmath_2} \,, \tag{5.70}$$

$$\boldsymbol{j}^D_{\mathrm{eff}}(\boldsymbol{q},t) = \frac{-e^2}{mc\Omega}\sum_{\imath,\boldsymbol{q}'}\sum_{\jmath_1\jmath_2} \boldsymbol{A}(\boldsymbol{q}-\boldsymbol{q}',t)\, e^{i\boldsymbol{q}'\,\boldsymbol{R}_\imath}\Big[\int d^3k \hat{f}^*_{\jmath_1}(\boldsymbol{k}+\boldsymbol{q}') \hat{f}_{\jmath_2}(\boldsymbol{k})\Big] D^\imath_{\jmath_1\jmath_2} \,. \tag{5.71}$$

As follows from (5.49) we only need to consider $\boldsymbol{j}^P_{\mathrm{eff}}(\boldsymbol{q},t)$ and $\boldsymbol{j}^D_{\mathrm{eff}}(\boldsymbol{q},t)$ in the limit $\boldsymbol{q}\to 0$. Using (5.55), (5.56) and (5.57) we obtain

$$\lim_{\boldsymbol{q}\to 0} \boldsymbol{j}^P_{\mathrm{eff}}(\boldsymbol{q},t) = \lim_{\boldsymbol{q}\to 0}\left\{\frac{-\imath e\hbar}{2m\sqrt{\alpha}}\sum_{\imath,\hat{\boldsymbol{\xi}}} \hat{\boldsymbol{\xi}}\, e^{i\boldsymbol{q}\,\boldsymbol{R}_\imath} P^\imath_{\hat{\boldsymbol{\xi}}}\right\} \,, \tag{5.72}$$

$$\lim_{\boldsymbol{q}\to 0} \boldsymbol{j}^D_{\mathrm{eff}}(\boldsymbol{q},t) = \lim_{\boldsymbol{q}\to 0}\left\{\frac{-e^2}{mc\Omega}\sum_{\imath,\boldsymbol{q}'} \boldsymbol{A}(\boldsymbol{q}-\boldsymbol{q}',t)\, e^{i\boldsymbol{q}'\,\boldsymbol{R}_\imath}\left[1+\chi_0(\boldsymbol{q}') + \sum_{M=1}^{\infty}\sum_{\hat{\boldsymbol{\xi}}_1\ \hat{\boldsymbol{\xi}}_M} \chi_{\hat{\boldsymbol{\xi}}_1\ \hat{\boldsymbol{\xi}}_M}(\boldsymbol{q}')\, S^\imath_{\hat{\boldsymbol{\xi}}_1} S^\imath_{\hat{\boldsymbol{\xi}}_2} \ldots S^\imath_{\hat{\boldsymbol{\xi}}_M}\right]\right\} \,. \tag{5.73}$$

In terms of the boson operators these expressions read

$$\lim_{\boldsymbol{q}\to 0} \boldsymbol{\jmath}^{P}_{\mathrm{eff}}(\boldsymbol{q},t) = \lim_{\boldsymbol{q}\to 0} \left\{ \frac{-ie\hbar\sqrt{2N}}{2m} \sum_{\lambda} \boldsymbol{\varepsilon}_{\boldsymbol{q}\lambda} \sqrt{\frac{2m\omega_{\boldsymbol{q}\lambda}}{\hbar}} \left[A_{\boldsymbol{q}\lambda} - A^{+}_{-\boldsymbol{q}\lambda} \right] \right\} , \tag{5.74}$$

$$\begin{aligned} \lim_{\boldsymbol{q}\to 0} \boldsymbol{\jmath}^{D}_{\mathrm{eff}}(\boldsymbol{q},t) = \lim_{\boldsymbol{q}\to 0} \Bigg\{ \frac{-2Ne^2}{mc\Omega} \sum_{\boldsymbol{K}_n} \Bigg[& \boldsymbol{A}(\boldsymbol{q}-\boldsymbol{K}_n,t)[1+\chi_0(\boldsymbol{K}_n)] \\ & + \sum_{M=1}^{\infty} \sum_{\hat{\boldsymbol{\xi}}_1 \cdots \hat{\boldsymbol{\xi}}_M} \sum_{\boldsymbol{k}_1 \cdots \boldsymbol{k}_M, \lambda_1 \cdots \lambda_M} \boldsymbol{A}(\boldsymbol{q}-\boldsymbol{K}_n-(\boldsymbol{k}_1+\ldots+\boldsymbol{k}_M),t) \Bigg[\\ & \chi_{\hat{\boldsymbol{\xi}}_1 \cdots \hat{\boldsymbol{\xi}}_M}(\boldsymbol{K}_n+\boldsymbol{k}_1+\ldots+\boldsymbol{k}_M) \prod_{j=1}^{M} \sqrt{\frac{\hbar}{4Nm\alpha\omega_{\boldsymbol{k}_j\lambda_j}}} \boldsymbol{\varepsilon}_{\boldsymbol{k}_j\lambda_j} \cdot \hat{\boldsymbol{\xi}}_j (A^{+}_{\boldsymbol{k}_j\lambda_j} + A_{-\boldsymbol{k}_j\lambda_j}) \Bigg] \Bigg] \Bigg] \Bigg\} . \end{aligned} \tag{5.75}$$

The macroscopic quantity $\lim_{\boldsymbol{q}\to 0} \boldsymbol{\jmath}(\boldsymbol{q},\omega)$, that appears in the criterion (5.49) for the Meissner-Ochsenfeld effect, can now be calculated provided that $\boldsymbol{A}(\boldsymbol{q},t)$ is interpreted as a Fourier component of the macroscopic field. This interpretation implies

$$\lim_{\boldsymbol{q}\to 0} \boldsymbol{A}(\boldsymbol{q}+\boldsymbol{K}_n,t) = 0 \qquad \text{for} \qquad \boldsymbol{K}_n \neq 0 . \tag{5.76}$$

The calculation goes as follows. Up to linear order in the field $\boldsymbol{A}(\boldsymbol{q},t)$ the Fourier component $\boldsymbol{\jmath}(\boldsymbol{q},t)$ of the macroscopic current density is given by

$$\boldsymbol{\jmath}(\boldsymbol{q},t) = \boldsymbol{\jmath}^{P}(\boldsymbol{q},t) + \boldsymbol{\jmath}^{D}(\boldsymbol{q},t) \tag{5.77}$$

with

$$\boldsymbol{\jmath}^{P}(\boldsymbol{q},t) = \lim_{\varepsilon\to 0} \frac{1}{i\hbar} \int_{-\infty}^{t} d\tau\, e^{\varepsilon\tau} \langle [\boldsymbol{\jmath}^{P}_{\mathrm{eff}}(\boldsymbol{q},t), H(1)_{\mathrm{eff}}(\tau)] \rangle \tag{5.78}$$

and

$$\boldsymbol{\jmath}^{D}(\boldsymbol{q},t) = \langle \boldsymbol{\jmath}^{D}_{\mathrm{eff}}(\boldsymbol{q},t) \rangle . \tag{5.79}$$

The thermal average $\langle \ldots \rangle$ is taken with respect to the eigenstates $|\varphi_n\rangle$ of $H(0)_{\mathrm{eff}}$, i.e.

$$\langle \ldots \rangle = \left[\sum_{n} e^{-\beta E_n} \right]^{-1} \left[\sum_{n} e^{-\beta E_n} \langle \varphi_n | \ldots | \varphi_n \rangle \right] , \tag{5.80}$$

with E_n being the energy corresponding with $|\varphi_n\rangle$. The expression (5.78) has been derived by Kubo [19] using linear response theory. The factor $e^{\varepsilon\tau}$ in the integrand indicates that the field is switched on adiabatically. Substituting the expressions (5.62), (5.74) and (5.75) into (5.78) and (5.79), respectively, and using (5.57), (5.66) and (5.76) we arrive at

$$\lim_{\boldsymbol{q}\to 0} \boldsymbol{\jmath}^P(\boldsymbol{q},t) = \lim_{\boldsymbol{q}\to 0}\lim_{\varepsilon\to 0} \frac{Ne^2}{mc\Omega} \sum_{\boldsymbol{k}\lambda\lambda'} \boldsymbol{\varepsilon}_{\boldsymbol{q}\lambda'} \hbar\sqrt{\omega_{\boldsymbol{k}\lambda}\omega_{\boldsymbol{q}\lambda'}} \int_{-\infty}^{\infty} d\tau\, e^{\varepsilon\tau} \boldsymbol{A}(\boldsymbol{k},\tau)\cdot\boldsymbol{\varepsilon}_{\boldsymbol{k}\lambda} G_1(t-\tau), \quad (5.81)$$

where $G_1(t-\tau)$ is a retarded Green function, given by

$$G_1(t) = -\frac{i}{\hbar}\,\theta(t)\langle[A_{\boldsymbol{q}\lambda'}(t) - A^+_{-\boldsymbol{q}\lambda'}(t), A_{\boldsymbol{k}\lambda} - A^+_{-\boldsymbol{k}\lambda}]\rangle\ , \quad (5.82)$$

and

$$\lim_{\boldsymbol{q}\to 0} \boldsymbol{\jmath}^D(\boldsymbol{q},t) = -\lim_{\boldsymbol{q}\to 0} \frac{2Ne^2}{mc\Omega}\boldsymbol{A}(\boldsymbol{q},t)\ . \quad (5.83)$$

Consequently the Fourier transforms $\boldsymbol{\jmath}(\boldsymbol{q},\omega)$ and $\boldsymbol{A}(\boldsymbol{q},\omega)$, as given by (5.50), satisfy the following relation:

$$\lim_{\boldsymbol{q}\to 0}\lim_{\omega\to 0} \boldsymbol{\jmath}(\boldsymbol{q},\omega) = \lim_{\boldsymbol{q}\to 0}\lim_{\omega\to 0}\lim_{\varepsilon\to 0} \frac{2Ne^2}{mc\Omega}\left[-\boldsymbol{A}(\boldsymbol{q},\omega) + \frac{1}{2}\sum_{\boldsymbol{k}\lambda\lambda'} \boldsymbol{\varepsilon}_{\boldsymbol{q}\lambda'}\hbar\sqrt{\omega_{\boldsymbol{k}\lambda}\omega_{\boldsymbol{q}\lambda'}}\,\boldsymbol{A}(\boldsymbol{k},\omega)\,G_1(\omega+i\varepsilon)\right]\ , \quad (5.84)$$

with

$$G_1(\omega) = \int_{-\infty}^{\infty} dt\, G_1(t)\, e^{i\omega t}\ . \quad (5.85)$$

The final step of the calculation consists of determining the Fourier transform $G_1(\omega)$ of the retarded Green function (5.82) in the limit $\omega \to 0$. This is done by using the equations of motion for the retarded Green functions. The relevant equations of motion are

$$\begin{aligned} i\hbar\frac{dG_1(t)}{dt} &= \frac{-i}{\hbar}\,\theta(t)\langle\Big[[A_{\boldsymbol{q}\lambda'}(t) - A^+_{-\boldsymbol{q}\lambda'}(t), H(0)_{\text{eff}}], A_{\boldsymbol{k}\lambda} - A^+_{-\boldsymbol{k}\lambda}\Big]\rangle \\ &= \hbar\omega_{\boldsymbol{q}\lambda'}\,G_2(t) + \sum_{M=3}^{\infty} 2M\Big\{ \end{aligned}$$

$$N \sum_{\boldsymbol{K}_n} \sum_{\boldsymbol{R}_i \neq 0} \sum_{\boldsymbol{q}_0}{}' e^{i\boldsymbol{q}_0 \cdot \boldsymbol{R}_i} \frac{4\pi e^2}{\Omega q_0^2} e^{-\alpha q_0^2} \frac{i^M}{M!} \sum_{\substack{\boldsymbol{k}_1 \ldots \boldsymbol{k}_M \\ \lambda_1 \ldots \lambda_M}} \delta_{\boldsymbol{k}_1 + \ldots + \boldsymbol{k}_M, \boldsymbol{K}_n} \prod_{j=1}^{M} \Bigg[\sqrt{\frac{\hbar}{4Nm\omega_{\boldsymbol{k}_j \lambda_j}}}\, \boldsymbol{\varepsilon}_{\boldsymbol{k}_j \lambda_j} \cdot \boldsymbol{q}_0 \left[e^{-i\boldsymbol{k}_j \cdot \boldsymbol{R}_i} - 1 \right] \Bigg] \delta_{\boldsymbol{k}_1 \boldsymbol{q}} \, G_M(t) \Bigg\} \tag{5.86}$$

and

$$i\hbar \frac{dG_2(t)}{dt} = -2\delta(t) \delta_{-\boldsymbol{k}\boldsymbol{q}} \, \delta_{\lambda\lambda'} + \hbar\omega_{\boldsymbol{q}\lambda'} \, G_1(t) \, , \tag{5.87}$$

where the retarded Green functions $G_2(t)$ and $G_M(t)$ are given by

$$\begin{aligned} G_2(t) &= -\frac{i}{\hbar} \theta(t) \langle [A_{\boldsymbol{q}\lambda'}(t) + A^+_{-\boldsymbol{q}\lambda'}(t), A_{\boldsymbol{k}\lambda} - A^+_{-\boldsymbol{k}\lambda}] \rangle \, , \\ G_M(t) &= -\frac{i}{\hbar} \theta(t) \langle [\prod_{j=2}^{M} (A^+_{\boldsymbol{k}_j \lambda_j} + A_{-\boldsymbol{k}_j \lambda_j})(t), A_{\boldsymbol{k}\lambda} - A^+_{-\boldsymbol{k}\lambda}] \rangle \, . \end{aligned} \tag{5.88}$$

The corresponding relations between the Fourier transforms $G_1(\omega)$, $G_2(\omega)$ and $G_M(\omega)$ can easily be calculated. Eliminating $G_2(\omega)$ we arrive at

$$\begin{aligned} G_1(\omega) = \frac{1}{\hbar[\omega^2 - \omega^2_{\boldsymbol{q}\lambda}]} \Bigg[& -2\omega_{\boldsymbol{q}\lambda} \, \delta_{-\boldsymbol{k}\boldsymbol{q}} \, \delta_{\lambda\lambda'} + \omega \sum_{M=3}^{\infty} 2M \Bigg\{ \\ & N \sum_{\boldsymbol{K}_n} \sum_{\boldsymbol{R}_i \neq 0} \sum_{\boldsymbol{q}_0}{}' e^{i\boldsymbol{q}_0 \boldsymbol{R}_i} \frac{4\pi e^2}{\Omega q_0^2} e^{-\alpha q_0^2} \frac{i^M}{M!} \sum_{\substack{\boldsymbol{k}_1 \ldots \boldsymbol{k}_M \\ \lambda_1 \ldots \lambda_M}} \delta_{\boldsymbol{k}_1 + \ldots + \boldsymbol{k}_M, \boldsymbol{K}_n} \prod_{j=1}^{M} \Bigg[\\ & \sqrt{\frac{\hbar}{4Nm\omega_{\boldsymbol{k}_j \lambda_j}}}\, \boldsymbol{\varepsilon}_{\boldsymbol{k}_j \lambda_j} \cdot \boldsymbol{q}_0 [e^{-i\boldsymbol{k}_j \cdot \boldsymbol{R}_i} - 1] \Bigg] \delta_{\boldsymbol{k}_1 \boldsymbol{q}} \, G_M(\omega) \Bigg\} \Bigg] \, . \end{aligned} \tag{5.89}$$

The Fourier transform $G_M(\omega)$ of the Green function $G_M(t)$, given by (5.88), is a very complicated function of ω. A formal expression, however, can be obtained from (5.80):

$$\begin{aligned} G_M(\omega + i\varepsilon) = \frac{1}{\hbar} \Bigg[\sum_n e^{-\beta E_n} \Bigg]^{-1} \Bigg[\sum_{n,m} e^{-\beta E_n} \Bigg\{ \\ \langle \varphi_n | \prod_{j=2}^{M} (A^+_{\boldsymbol{k}_j \lambda_j} + A_{-\boldsymbol{k}_j \lambda_j}) | \varphi_m \rangle \langle \varphi_m | A_{\boldsymbol{k}\lambda} - A^+_{-\boldsymbol{k}\lambda} | \varphi_n \rangle \left[\omega + i\varepsilon + \frac{E_n - E_m}{\hbar} \right]^{-1} \end{aligned}$$

$$- \langle\varphi_n|A_{\boldsymbol{k}\lambda} - A^+_{-\boldsymbol{k}\lambda}|\varphi_m\rangle\langle\varphi_m|\prod_{j=2}^{M}(A^+_{\boldsymbol{k}_j\lambda_j} + A_{-\boldsymbol{k}_j\lambda_j})|\varphi_n\rangle \left[\omega + i\varepsilon + \frac{E_m - E_n}{\hbar}\right]^{-1}\Bigg\}\Bigg] \,, \tag{5.90}$$

where use is made of the identities

$$\begin{aligned}
&\langle\varphi_n|\left[\prod_{j=2}^{M}(A^+_{\boldsymbol{k}_j\lambda_j} + A_{-\boldsymbol{k}_j\lambda_j})(t)\right]\left[A_{\boldsymbol{k}\lambda} - A^+_{-\boldsymbol{k}\lambda}\right]|\varphi_n\rangle \\
&\quad = \sum_m \langle\varphi_n|\left[\prod_{j=2}^{M}(A^+_{\boldsymbol{k}_j\lambda_j} + A_{-\boldsymbol{k}_j\lambda_j})(t)\right]|\varphi_m\rangle\langle\varphi_m|A_{\boldsymbol{k}\lambda} - A^+_{-\boldsymbol{k}\lambda}|\varphi_n\rangle \\
&\quad = \sum_m e^{i(\frac{E_n - E_m}{\hbar})t}\,\langle\varphi_n|\left[\prod_{j=2}^{M}(A^+_{\boldsymbol{k}_j\lambda_j} + A_{-\boldsymbol{k}_j\lambda_j})\right]|\varphi_m\rangle\langle\varphi_m|A_{\boldsymbol{k}\lambda} - A^+_{-\boldsymbol{k}\lambda}|\varphi_n\rangle
\end{aligned} \tag{5.91}$$

and

$$-i\int_{-\infty}^{\infty} dt\,\theta(t)\,e^{i(\omega+i\varepsilon)t}\,e^{i(\frac{E_n - E_m}{\hbar})t} = \left[\omega + i\varepsilon + \frac{E_n - E_m}{\hbar}\right]^{-1} . \tag{5.92}$$

After rewriting (5.90) as

$$\begin{aligned}
G_M(\omega+i\varepsilon) = \frac{1}{\hbar}\left[\sum_n e^{-\beta E_n}\right]^{-1}\Bigg[\sum_{n,m}\Big[e^{-\beta E_n} - e^{-\beta E_m}\Big]\Bigg\{ \\
\langle\varphi_n|\prod_{j=2}^{M}(A^+_{\boldsymbol{k}_j\lambda_j} + A_{-\boldsymbol{k}_j\lambda_j})|\varphi_m\rangle\langle\varphi_m|A_{\boldsymbol{k}\lambda} - A^+_{-\boldsymbol{k}\lambda}|\varphi_n\rangle\left[\omega + i\varepsilon + \frac{E_n - E_m}{\hbar}\right]^{-1}\Bigg\}\Bigg]
\end{aligned} \tag{5.93}$$

we obtain

$$\lim_{\omega\to 0}\lim_{\varepsilon\to 0}(\omega + i\varepsilon)G_M(\omega+i\varepsilon) = 0 \,. \tag{5.94}$$

Substituting (5.89) and (5.94) into (5.84) we finally arrive at the decisive relation between $\boldsymbol{\jmath}(\boldsymbol{q},\omega)$ and $\boldsymbol{A}(\boldsymbol{q},\omega)$:

$$\begin{aligned}
\lim_{\boldsymbol{q}\to 0}\lim_{\omega\to 0}\boldsymbol{\jmath}(\boldsymbol{q},\omega) &= \lim_{\boldsymbol{q}\to 0}\lim_{\omega\to 0}\frac{2Ne^2}{mc\Omega}\left[-\boldsymbol{A}(\boldsymbol{q},\omega) + \boldsymbol{A}(-\boldsymbol{q},\omega)\right] \\
&= -\lim_{\boldsymbol{q}\to 0}\lim_{\omega\to 0}\frac{2Ne^2}{mc\Omega}\left[2i\,\mathrm{Im}\,(\boldsymbol{A}(\boldsymbol{q},\omega))\right] \,.
\end{aligned} \tag{5.95}$$

Now we can directly conclude that the low-density electron system does not show a Meissner-Ochsenfeld effect as the imaginary part of $\boldsymbol{A}(\boldsymbol{q},\omega)$ disappears in the limit $\boldsymbol{q}\to 0$.

We wish to remark that the present conclusion only holds for sufficiently low densities where the effect of exchange can be neglected. This neglect, however, does not automatically mean that the appearance of a Meissner-Ochsenfeld effect could be excluded a priori, for the ground state of the low-density system is highly correlated. Apparently the electron-electron correlation, which is described by the effective Hamiltonian $\widetilde{H}_{\text{eff}}$ given by (5.59), does not give the necessary rigidity to the system's wave function for resisting the magnetic field [20]. This absence of sufficient rigidity in the low-density system does not follow a priori from a general argument, as far as we know. Likewise the effect of the exchange on the rigidity cannot be predicted. Consequently the question is still open whether the model shows a Meissner-Ochsenfeld effect at higher densities.

6. Conclusions

In this paper the low-density electron system has been studied within a purely quantum-mechanical context. It appears that the semi classical approaches of Wigner and Carr can be justified. The results of Wigner's approach of the low-density electron system are identical to those of a Hartree-Fock theory with the ground state being a Slater determinant of $2N$ harmonic oscillator ground state functions localized at the sites of a regular lattice (section 3). The effect of exchange has been considered as well leading to the conclusion that a ferromagnetic lattice is favourable to an antiferromagnetic lattice for $r_s \geq 14$.

In order to reproduce the results of Carr's approach the quantummechanical calculation must take into account the effect of electron-electron correlation (section 4). Now the eigenstates are expressed as linear combinations of all possible Slater determinants of $2N$ harmonic oscillator eigenfunctions, localized at the sites of the Wigner lattice. An important result of the theory is the existence of an effective free boson Hamiltonian generating the exact eigenstates and energy spectrum up to order $r_s^{-3/2}$. The appearing boson operators have been expressed completely in terms of the original fermion operators.

The implications of the approach, as developed in section 4, are not restricted to the low-density electron system only. Any lattice of atoms or ions can be treated in exactly the same way as the Wigner lattice of electrons. The results, obtained by neglecting the effect of exchange, are then identical to those of Born's lattice theory. Thus we have completely justified Born's lattice theory from a quantummechanical point of view.

Finally the approach of section 4 has been applied to the jellium model in a magnetic field (section 5). By way of calculating the current density we have shown that the low-density jellium model allows a homogeneous internal magnetic field. The eventual appearance of a Meissner-Ochsenfeld effect has also been discussed, the conclusion being negative for a low-density system.

Appendix I

Substitution of (3.7) into (3.4) gives the Hartree-Fock energy of the Wigner lattice

$$E_{HF} = |C|^2 \langle | d_{\tau_{2N}}(\boldsymbol{R}_{2N}) \dots d_{\tau_1}(\boldsymbol{R}_1) H \, d^+_{\tau_1}(\boldsymbol{R}_1) \dots d^+_{\tau_{2N}}(\boldsymbol{R}_{2N}) | \rangle \tag{I.1}$$

with

$$|C|^{-2} = \langle | d_{\tau_{2N}}(\boldsymbol{R}_{2N}) \dots d_{\tau_1}(\boldsymbol{R}_1) d^+_{\tau_1}(\boldsymbol{R}_1) \dots d^+_{\tau_{2N}}(\boldsymbol{R}_{2N}) | \rangle \ . \tag{I.2}$$

In order to calculate E_{HF} explicitly we use

$$H d^+_{\tau_1}(\boldsymbol{R}_1) \dots d^+_{\tau_{2N}}(\boldsymbol{R}_{2N}) | \rangle =$$

$$\sum_{i=1}^{2N} d^+_{\tau_1}(\boldsymbol{R}_1) \dots d^+_{\tau_{i-1}}(\boldsymbol{R}_{i-1}) \, [H, d^+_{\tau_i}(\boldsymbol{R}_i)] \, d^+_{\tau_{i+1}}(\boldsymbol{R}_{i+1}) \dots d^+_{\tau_{2N}}(\boldsymbol{R}_{2N}) | \rangle \ , \tag{I.3}$$

whose validity directly follows from $H|\rangle = 0$. Next we rewrite (I.3) as

$$H d^+_{\tau_1}(\boldsymbol{R}_1) \dots d^+_{\tau_{2N}}(\boldsymbol{R}_{2N}) | \rangle =$$

$$\sum_{i=1}^{2N} \sum_{j=i+1}^{2N} (-1)^{-i+j+1} \left(\prod_{m \neq i,j} d^+_{\tau_m}(\boldsymbol{R}_m) \right) \left\{ [H, d^+_{\tau_i}(\boldsymbol{R}_i)], d^+_{\tau_j}(\boldsymbol{R}_j) \right\} | \rangle +$$

$$\sum_{i=1}^{2N} (-1)^{2N-i} \left(\prod_{m \neq i} d^+_{\tau_m}(\boldsymbol{R}_m) \right) [H, d^+_{\tau_i}(\boldsymbol{R}_i)] | \rangle \ . \tag{I.4}$$

Substituting (I.4) into (I.1) and using

$$\begin{aligned} d_{\tau_{2N}}(\boldsymbol{R}_{2N}) \dots d_{\tau_1}(\boldsymbol{R}_1) &= (-1)^{2N-i} d_{\tau_i}(\boldsymbol{R}_i) \left(\prod_{m \neq i} d^+_{\tau_m}(\boldsymbol{R}_m) \right)^+ \\ &= (-1)^{i-j-1} d_{\tau_j}(\boldsymbol{R}_j) d_{\tau_i}(\boldsymbol{R}_i) \left(\prod_{m \neq i,j} d^+_{\tau_m}(\boldsymbol{R}_m) \right)^+ \ , \end{aligned} \tag{I.5}$$

we arrive at

$$E_{HF} = |C|^2 \sum_{i=1}^{2N} \langle | d_{\tau_i}(\boldsymbol{R}_i) \left(\prod_{m \neq i} d^+_{\tau_m}(\boldsymbol{R}_m) \right)^+ \left(\prod_{m \neq i} d^+_{\tau_m}(\boldsymbol{R}_m) \right) [H, d^+_{\tau_i}(\boldsymbol{R}_i)] | \rangle$$

$$+ \quad |C|^2 \sum_{i=1}^{2N} \sum_{j=i+1}^{2N} \langle | d_{\tau_j}(\boldsymbol{R}_j) d_{\tau_i}(\boldsymbol{R}_i) \left(\prod_{m \neq i,j} d^+_{\tau_m}(\boldsymbol{R}_m) \right)^+ \left(\prod_{m \neq i,j} d^+_{\tau_m}(\boldsymbol{R}_m) \right)$$

$$\times \quad \left\{ [H, d^+_{\tau_i}(\boldsymbol{R}_i)], d^+_{\tau_j}(\boldsymbol{R}_j) \right\} | \rangle \ . \tag{I.6}$$

Now Wick's theorem can directly be applied to this expression, as the following relations hold:

$$[H, d^+_{\tau_i}(\boldsymbol{R}_i)] | \rangle = \left[\frac{(2\pi)^3}{\Omega} \right]^{1/2} \sum_{\boldsymbol{k}} \frac{\hbar^2 k^2}{2m} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_i} \hat{f}^*(\boldsymbol{k}) c^+_{\boldsymbol{k}\tau_i} | \rangle \ , \tag{I.7}$$

$$\{ [H, d^+_{\tau_i}(\boldsymbol{R}_i)], d^+_{\tau_j}(\boldsymbol{R}_j) \} =$$

$$\frac{(2\pi)^3}{\Omega} \sum_{\boldsymbol{q}}{}' \sum_{\boldsymbol{k},\boldsymbol{k}'} V(\boldsymbol{q}) \hat{f}^*(\boldsymbol{k}-\boldsymbol{q}) \hat{f}^*(\boldsymbol{k}'+\boldsymbol{q}) e^{-i(\boldsymbol{k}-\boldsymbol{q})\cdot\boldsymbol{R}_i} e^{-i(\boldsymbol{k}'+\boldsymbol{q})\boldsymbol{R}_j} c^+_{\boldsymbol{k}\tau_i} c^+_{\boldsymbol{k}'\tau_j} \ . \tag{I.8}$$

The resulting expression for E_{HF} is given by

$$\begin{aligned} E_{HF} \quad &= \quad |C|^2 \sum_{\lambda} \mathrm{sgn}(\lambda) \sum_{i=1}^{2N} \delta_{\tau_i \tau_{\lambda(i)}} K(\boldsymbol{R}_i - \boldsymbol{R}_{\lambda(i)}) \prod_{m \neq i} S(\boldsymbol{R}_m - \boldsymbol{R}_{\lambda(m)}) \delta_{\tau_m \tau_{\lambda(m)}} \\ &+ \quad |C|^2 \sum_{\lambda} \mathrm{sgn}(\lambda) \frac{1}{2} \sum_{i \neq j} \delta_{\tau_i \tau_{\lambda(i)}} \delta_{\tau_j \tau_{\lambda(j)}} \Bigg[\\ &\qquad P(\boldsymbol{R}_i - \boldsymbol{R}_{\lambda(i)}; \boldsymbol{R}_j - \boldsymbol{R}_{\lambda(j)}; \boldsymbol{R}_i - \boldsymbol{R}_j) \prod_{m \neq i} S(\boldsymbol{R}_m - \boldsymbol{R}_{\lambda(m)}) \delta_{\tau_m \tau_{\lambda(m)}} \Bigg] \end{aligned} \tag{I.9}$$

with

$$|C|^{-2} = \sum_{\lambda} \mathrm{sgn}(\lambda) \prod_{m} S(\boldsymbol{R}_m - \boldsymbol{R}_{\lambda(m)}) \delta_{\tau_m \tau_{\lambda(m)}} \ , \tag{I.10}$$

where the sum over λ runs over all $(2N)!$ permutations of $1, 2, \ldots, 2N$. The function S denotes the overlap, whereas the functions K and P are related to the kinetic and potential energy respectively:

$$S(\boldsymbol{R}_i - \boldsymbol{R}_{\lambda(i)}) = \{ d_\uparrow(\boldsymbol{R}_{\lambda(i)}), d^+_\uparrow(\boldsymbol{R}_i) \} = \int d^3k \, \hat{f}(\boldsymbol{k}) \hat{f}^*(\boldsymbol{k}) e^{-i\boldsymbol{k}\cdot(\boldsymbol{R}_i - \boldsymbol{R}_{\lambda(i)})} \tag{I.11}$$

$$K(\boldsymbol{R}_i - \boldsymbol{R}_{\lambda(i)}) = \langle | d_\uparrow(\boldsymbol{R}_{\lambda(i)}) [H, d^+_\uparrow(\boldsymbol{R}_i)] | \rangle = \int d^3k \, \frac{\hbar^2 k^2}{2m} \hat{f}(\boldsymbol{k}) \hat{f}^*(\boldsymbol{k}) e^{-i\boldsymbol{k}\cdot(\boldsymbol{R}_i - \boldsymbol{R}_{\lambda(i)})} \tag{I.12}$$

$$P(\boldsymbol{R}_i - \boldsymbol{R}_{\lambda(i)}; \boldsymbol{R}_j - \boldsymbol{R}_{\lambda(j)}; \boldsymbol{R}_i - \boldsymbol{R}_j) = \langle |d_\downarrow(\boldsymbol{R}_{\lambda(j)}) d_\uparrow(\boldsymbol{R}_{\lambda(i)}) \{[H, d_\uparrow^+(\boldsymbol{R}_i)], d_\downarrow^+(\boldsymbol{R}_j)\}| \rangle$$

$$= {\sum_{\boldsymbol{q}}}' V(\boldsymbol{q})\ e^{-i\boldsymbol{q}\cdot(\boldsymbol{R}_i - \boldsymbol{R}_j)} \Big[\int d^3k d^3k'\, \hat{f}^*(\boldsymbol{k}' + \boldsymbol{q})\, \hat{f}^*(\boldsymbol{k} - \boldsymbol{q})\, \hat{f}(\boldsymbol{k}) \hat{f}(\boldsymbol{k}') e^{-i\boldsymbol{k}(\boldsymbol{R}_i - \boldsymbol{R}_{\lambda(i)})}\, e^{-i\boldsymbol{k}'(\boldsymbol{R}_j - \boldsymbol{R}_{\lambda(j)})} \Big] \tag{I.13}$$

Up to order $S(\boldsymbol{R}_i - \boldsymbol{R}_{\lambda(i)})^2$ only two terms, appearing in the sum over the permutations, are relevant. The first term corresponds with the identity permutation ($\lambda(i) = i$ for all i) and the second term with the sum over all permutations of the form $\lambda(i) = j$, $\lambda(j) = i$, $i \neq j$. Neglecting the remaining terms, i.e. considering only two-particle exchange contributions, we obtain

$$\begin{aligned} E_{HF} \;=\; & |C|^2 \Bigg\{ \sum_i S(0)^{2N-1} K(0) + \frac{1}{2} \sum_{i \neq j} S(0)^{2N-2} P(0; 0; \boldsymbol{R}_i - \boldsymbol{R}_j) \\ & - \Bigg[\sum_i \sum_{j \neq i} \delta_{\tau_i \tau_j} S(0)^{2N-2} [K(\boldsymbol{R}_i - \boldsymbol{R}_j) S(\boldsymbol{R}_j - \boldsymbol{R}_i) \\ & + \frac{1}{2} P(\boldsymbol{R}_i - \boldsymbol{R}_j; \boldsymbol{R}_j - \boldsymbol{R}_i; \boldsymbol{R}_i - \boldsymbol{R}_j)] \\ & + \sum_i \sum_{j \neq i} \sum_{m \neq i,j} \frac{1}{2} S(0)^{2N-3} [K(0) S(\boldsymbol{R}_j - \boldsymbol{R}_m)^2 \delta_{\tau_m \tau_j} \\ & + \delta_{\tau_i \tau_m} S(\boldsymbol{R}_m - \boldsymbol{R}_i) P(\boldsymbol{R}_i - \boldsymbol{R}_m; 0; \boldsymbol{R}_i - \boldsymbol{R}_j) \\ & + \delta_{\tau_j \tau_m} S(\boldsymbol{R}_m - \boldsymbol{R}_j) P(0; \boldsymbol{R}_j - \boldsymbol{R}_m; \boldsymbol{R}_i - \boldsymbol{R}_j)] \\ & + \sum_i \sum_{j \neq i} \sum_{m \neq i,j} \sum_{n \neq m,i,j} \frac{1}{4} \delta_{\tau_m \tau_n} S(0)^{2N-4} S(\boldsymbol{R}_m - \boldsymbol{R}_n)^2 P(0; 0; \boldsymbol{R}_i - \boldsymbol{R}_j) \Bigg] \Bigg\}\ , \end{aligned} \tag{I.14}$$

where

$$|C|^2 = \left[S(0)^{2N} - \frac{1}{2} \sum_m \sum_{n \neq m} S(\boldsymbol{R}_m - \boldsymbol{R}_n)^2 \, S(0)^{2N-2} \, \delta_{\tau_m \tau_n} \right]^{-1}$$
$$= S(0)^{2N} + \frac{1}{2} \sum_m \sum_{n \neq m} S(\boldsymbol{R}_m - \boldsymbol{R}_n)^2 \, S(0)^{2N-2} \, \delta_{\tau_m \tau_n} \, . \qquad \text{(I.15)}$$

Thus the first term in the expansion is

$$E_{HF}(0) = 2N \, K(0) + \frac{1}{2} \sum_{i \neq j} P(0;0;\boldsymbol{R}_i - \boldsymbol{R}_j) \, , \qquad \text{(I.16)}$$

where we have used that $S(0) = 1$. This expression, together with (I.12) and (I.13), gives the Hartree energy (3.14). The next term is of order $S(\boldsymbol{R}_i - \boldsymbol{R}_j)^2$ and given by

$$\begin{aligned}
\Delta E_{HF} &= \sum_i \sum_{j \neq i} \delta_{\tau_i \tau_j} [K(0) S(\boldsymbol{R}_j - \boldsymbol{R}_i)^2 - K(\boldsymbol{R}_i - \boldsymbol{R}_j) S(\boldsymbol{R}_j - \boldsymbol{R}_i) \\
&+ \frac{1}{2} P(0;0;\boldsymbol{R}_i - \boldsymbol{R}_j) S(\boldsymbol{R}_i - \boldsymbol{R}_j)^2 - \frac{1}{2} P(\boldsymbol{R}_i - \boldsymbol{R}_j; \boldsymbol{R}_j - \boldsymbol{R}_i; \boldsymbol{R}_i - \boldsymbol{R}_j)] \\
&+ \frac{1}{2} \sum_i \sum_j \sum_{m \neq i,j} [\delta_{\tau_i \tau_m} P(0;0;\boldsymbol{R}_i - \boldsymbol{R}_j) S(\boldsymbol{R}_i - \boldsymbol{R}_m)^2 \\
&- \delta_{\tau_i \tau_m} P(\boldsymbol{R}_i - \boldsymbol{R}_m; 0; \boldsymbol{R}_i - \boldsymbol{R}_j) S(\boldsymbol{R}_m - \boldsymbol{R}_i) \\
&+ \delta_{\tau_j \tau_m} P(0;0;\boldsymbol{R}_i - \boldsymbol{R}_j) S(\boldsymbol{R}_j - \boldsymbol{R}_m)^2 \\
&- \delta_{\tau_j \tau_m} P(0; \boldsymbol{R}_j - \boldsymbol{R}_m; \boldsymbol{R}_i - \boldsymbol{R}_j) S(\boldsymbol{R}_m - \boldsymbol{R}_j)] \, . \qquad \text{(I.17)}
\end{aligned}$$

The magnitude of ΔE_{HF} depends on the spin configuration of the electron lattice. For a ferromagnetic spin state, i.e. $\tau_n = \uparrow$ or $\tau_n = \downarrow$ for all $n = 1, 2, \ldots, 2N$ we get

$$\begin{aligned}
\Delta E^f_{HF} &= \sum_{\boldsymbol{R}_n \neq 0} 2N [K(0) S(\boldsymbol{R}_n)^2 - K(\boldsymbol{R}_n) S(\boldsymbol{R}_n) \\
&- \frac{1}{2} P(\boldsymbol{R}_n; -\boldsymbol{R}_n; \boldsymbol{R}_n) + \frac{1}{2} P(0;0;\boldsymbol{R}_n) S(\boldsymbol{R}_n)^2] \\
&+ \sum_{\boldsymbol{R}_n \neq 0} \sum_{\boldsymbol{R}_m \neq \boldsymbol{R}_n, 0} 2N [P(0;0;\boldsymbol{R}_n) S(\boldsymbol{R}_m)^2 - P(\boldsymbol{R}_m; 0; \boldsymbol{R}_n) S(\boldsymbol{R}_m)] \, .
\end{aligned} \qquad \text{(I.18)}$$

For an antiferromagnetic spin state, i.e. $\tau_n = \uparrow$ for all electrons localized at the sublattice sites $\boldsymbol{R}_n$ $(n = 1, \ldots, N)$ and $\tau_n = \downarrow$ for all electrons localized at $\boldsymbol{R}_n + \boldsymbol{\delta}$ $(n = 1, \ldots, N)$, ΔE_{HF} is given by

$$\begin{aligned}
\Delta E^a_{HF} &= \sum_{\boldsymbol{R}_n \neq 0} 2N[K(0)S(\boldsymbol{R}_n)^2 - K(\boldsymbol{R}_n)S(\boldsymbol{R}_n) \\
&- \frac{1}{2}P(\boldsymbol{R}_n; -\boldsymbol{R}_n; \boldsymbol{R}_n) + \frac{1}{2}P(0;0;\boldsymbol{R}_n)S(\boldsymbol{R}_n)^2] \\
&+ \sum_{\boldsymbol{R}_n \neq 0} \sum_{\boldsymbol{R}_m \neq \boldsymbol{R}_n, 0} 2N[P(0;0;\boldsymbol{R}_n)S(\boldsymbol{R}_m)^2 - P(\boldsymbol{R}_m;0;\boldsymbol{R}_n)S(\boldsymbol{R}_m)] \\
&+ \sum_{\boldsymbol{R}_n} \sum_{\boldsymbol{R}_m \neq 0} 2N[P(0;0;\boldsymbol{R}_n + \boldsymbol{\delta})S(\boldsymbol{R}_m)^2 - P(\boldsymbol{R}_m;0;\boldsymbol{R}_n + \boldsymbol{\delta})S(\boldsymbol{R}_m)] \,.
\end{aligned} \tag{I.19}$$

The unknown wave function $\hat{f}$, that appears in (I 11), (I.12) and (I.13), is determined by the minimization procedure as discussed in section 3. Using the resulting Gaussian wave packet (3.16) we obtain

$$S(\boldsymbol{R}_n) = e^{-R_n^2/8\alpha} \tag{I.20}$$

$$K(\boldsymbol{R}_n) = \frac{\hbar^2}{2m}\left[\frac{3}{4\alpha} - \frac{R_n^2}{16\alpha^2}\right] e^{-R_n^2/8\alpha} \tag{I.21}$$

$$P(\boldsymbol{R}_m;0;\boldsymbol{x}) = P(0;\boldsymbol{R}_m;-\boldsymbol{x}) = {\sum_{\boldsymbol{q}}}' V(\boldsymbol{q})\, e^{-\alpha q^2}\, e^{\imath \boldsymbol{q}\cdot(\boldsymbol{x} - \frac{1}{2}\boldsymbol{R}_m)}\, e^{-R_n^2/8\alpha} \,. \tag{I.22}$$

$$P(\boldsymbol{R}_n; -\boldsymbol{R}_n; \boldsymbol{R}_n) = {\sum_{\boldsymbol{q}}}' V(\boldsymbol{q})\, e^{-\alpha q^2}\, e^{-R_n^2/8\alpha} \,. \tag{I.23}$$

The ferromagnetic and antiferromagnetic exchange energies are then given by

$$\begin{aligned}
\Delta E^f_{HF} &= 2N \sum_{\boldsymbol{R}_n \neq 0} e^{-R_n^2/4\alpha}\left[\frac{\hbar^2 R_n^2}{32m\alpha^2} + {\sum_{\boldsymbol{q}}}' V(\boldsymbol{q})\, e^{-\alpha q^2}(e^{\frac{1}{2}\imath \boldsymbol{q}\cdot\boldsymbol{R}_n} - \frac{1}{2} - \frac{1}{2}e^{\imath \boldsymbol{q}\,\boldsymbol{R}_n})\right. \\
&\left. + \sum_{\boldsymbol{R}_m \neq 0} {\sum_{\boldsymbol{q}}}' V(\boldsymbol{q})\, e^{-\alpha q^2}(e^{\imath \boldsymbol{q}\,\boldsymbol{R}_m} - e^{\imath \boldsymbol{q}\cdot(\boldsymbol{R}_m - \frac{1}{2}\boldsymbol{R}_m)})\right]
\end{aligned} \tag{I.24}$$

$$\Delta E^a_{HF} = 2N \sum_{\boldsymbol{R}_n \neq 0} e^{-R_n^2/4\alpha} \left[\frac{\hbar^2 R_n^2}{32 m \alpha^2} + {\sum_{\boldsymbol{q}}}' V(\boldsymbol{q})\, e^{-\alpha q^2} (e^{\frac{1}{2} i \boldsymbol{q} \cdot \boldsymbol{R}_n} - \frac{1}{2} - \frac{1}{2} e^{i \boldsymbol{q} \cdot \boldsymbol{R}_n}) \right.$$
$$+ \sum_{\boldsymbol{R}_m \neq 0} {\sum_{\boldsymbol{q}}}' V(\boldsymbol{q})\, e^{-\alpha q^2} (e^{i \boldsymbol{q} \cdot \boldsymbol{R}_m} - e^{i \boldsymbol{q} \cdot (\boldsymbol{R}_m - \frac{1}{2} \boldsymbol{R}_n)})$$
$$\left. + \sum_{\boldsymbol{R}_m} {\sum_{\boldsymbol{q}}}' V(\boldsymbol{q})\, e^{-\alpha q^2} (e^{i \boldsymbol{q} \cdot (\boldsymbol{R}_m + \boldsymbol{\delta})} - e^{i \boldsymbol{q} \cdot (\boldsymbol{R}_m + \boldsymbol{\delta} - \frac{1}{2} \boldsymbol{R}_n)}) \right] . \qquad \text{(I.25)}$$

After performing the sums over $\boldsymbol{R}_m$ we arrive at the expressions (3.25) and (3.26) respectively.

Appendix II

The functional $E_H(f)$, as given in (3.14), can be rewritten as

$$E_H(f) = 2N \int d^3k \, \frac{\hbar^2 k^2}{2m} \hat{f}(\boldsymbol{k}) \hat{f}^*(\boldsymbol{k}) + \frac{1}{2} \sum_{m \neq n} U(\boldsymbol{R}_n - \boldsymbol{R}_m) - \lim_{\boldsymbol{q} \to 0} 2N^2 \tilde{V}(\boldsymbol{q}) \; , \quad \text{(II.1)}$$

where

$$\tilde{V}(\boldsymbol{q}) = \frac{4\pi e^2}{\Omega q^2} \left[\int d^3k \, \hat{f}(\boldsymbol{k} + \boldsymbol{q}) \, \hat{f}^*(\boldsymbol{k}) \right]^2 \; , \quad \text{(II.2)}$$

and

$$U(\boldsymbol{R}_n - \boldsymbol{R}_m) = \sum_{\boldsymbol{q}} \tilde{V}(\boldsymbol{q}) \exp[i\boldsymbol{q} \cdot (\boldsymbol{R}_n - \boldsymbol{R}_m)] \; . \quad \text{(II.3)}$$

This expression can be easily minimized provided that $U(\boldsymbol{R}_n - \boldsymbol{R}_m)$ is replaced by the true Coulomb potential. Then (II.1) reads

$$\begin{aligned} E_H(f) &= E_{Cl} + 2N \left\{ \int d^3k \, \hat{f}(\boldsymbol{k}) \hat{f}^*(\boldsymbol{k}) \frac{\hbar^2 k^2}{2m} \right. \\ &\quad \left. - N \lim_{\boldsymbol{q} \to 0} \frac{4\pi e^2}{\Omega q^2} \left(\left[\int d^3k \, \hat{f}(\boldsymbol{k} + \boldsymbol{q}) \hat{f}^*(\boldsymbol{k}) \right]^2 - 1 \right) \right\} \; , \end{aligned} \quad \text{(II.4)}$$

where the energy of the classical electron gas, E_{Cl}, is given by

$$E_{Cl} = \frac{1}{2} \sum_{m \neq n} \frac{e^2}{|\boldsymbol{R}_m - \boldsymbol{R}_n|} - \frac{N}{\Omega} \lim_{\boldsymbol{q} \to 0} \frac{4\pi e^2}{q^2} = \frac{2\pi e^2}{\Omega} \sum_{\boldsymbol{q}}{}' \sum_{m \neq n} \frac{1}{q^2} \exp[i\boldsymbol{q} \cdot (\boldsymbol{R}_m - \boldsymbol{R}_n)] \; . \quad \text{(II.5)}$$

It follows from the form of the expression (II.4) that $E_H(f)$ is minimized by a real and isotropic function. Consequently we can use the expansion:

$$\begin{aligned} \hat{f}(\boldsymbol{k} + \boldsymbol{q}) &= \hat{f}(k) + \boldsymbol{q} \cdot \boldsymbol{\nabla} \hat{f}(k) + \frac{1}{2} (\boldsymbol{q} \cdot \boldsymbol{\nabla})^2 \hat{f}(k) + \ldots \\ &= \hat{f}(k) + \frac{\boldsymbol{q} \cdot \boldsymbol{k}}{k} \hat{f}'(k) + \frac{1}{2} \left\{ \frac{(\boldsymbol{q} \cdot \boldsymbol{k})^2}{k^2} \hat{f}''(k) + \hat{f}'(k) \left[\frac{q^2}{k} - \frac{(\boldsymbol{q} \cdot \boldsymbol{k})^2}{k^3} \right] \right\} + \ldots \end{aligned} \quad \text{(II.6)}$$

with $\hat{f}'(k) = \frac{d\hat{f}}{dk}$ and $\hat{f}''(k) = \frac{d^2\hat{f}}{dk^2}$. Substituting (II.6) into (II.4) and using

$$\lim_{\boldsymbol{q} \to 0} \frac{4\pi e^2}{\Omega q^2} \left\{ \left[\int d^3k \hat{f}(\boldsymbol{k} + \boldsymbol{q}) \hat{f}^*(\boldsymbol{k}) \right]^2 - 1 \right\} = \frac{16\pi e^2}{3\Omega} \int_0^\infty k^2 dk [\hat{f}''(k) + \frac{2}{k} \hat{f}'(k)] \hat{f}(k) \quad \text{(II.7)}$$

we arrive at

$$E_H(f) = E_{Cl} + 2N\left\{4\pi\int_0^\infty k^2 dk\hat{f}(k)\left[\hat{f}(k)\frac{\hbar^2k^2}{2m} - \frac{4\pi e^2N}{3\Omega}(\hat{f}''(k) + \frac{2}{k}f'(k))\right]\right.$$

$$\left. - \lambda\left[4\pi\int_0^\infty k^2 dk\hat{f}(k)^2 - 1\right]\right\}, \qquad \text{(II.8)}$$

where the Lagrange multiplier λ has been introduced in order to take into account the normalization of $\hat{f}$. The function $\hat{f}$ is now determined by the Euler equation

$$\frac{d^2}{dk^2}\left(\frac{\partial\mathcal{L}}{\partial\hat{f}''}\right) - \frac{d}{dk}\left(\frac{\partial\mathcal{L}}{\partial\hat{f}'}\right) + \frac{\partial\mathcal{L}}{\partial\hat{f}} = 0\,, \qquad \text{(II.9)}$$

where

$$\mathcal{L} = 4\pi\left[(-\lambda k^2 + \frac{\hbar^2k^4}{2m})\hat{f}^2 - \frac{4\pi Ne^2}{3\Omega}(\hat{f}'' + \frac{2\hat{f}'}{k})k^2\hat{f}\right]. \qquad \text{(II.10)}$$

This means that f complies with the differential equation

$$\frac{4\pi}{3}\frac{Ne^2}{\Omega}\frac{d^2}{dk^2}(k\hat{f}) = \left[\frac{\hbar^2k^2}{2m} - \lambda\right](k\hat{f})\,. \qquad \text{(II.11)}$$

The normalized solution of (II.11) reads

$$\hat{f}_0(k) = \left[\frac{2\alpha}{\pi}\right]^{3/4} e^{-\alpha k^2} \qquad \text{(II.12)}$$

and the Lagrange multiplier is given by

$$\lambda = \frac{8\pi Ne^2\alpha}{\Omega} \qquad \text{(II.13)}$$

with

$$\alpha^2 = \frac{3\Omega}{32\pi N}\frac{\hbar^2}{me^2}\,. \qquad \text{(II.14)}$$

The real space wave function f_0, which is the Fourier transform of (II.12), is given in (3.16).

It should be remarked that the approximation of replacing $U(\boldsymbol{R}_n - \boldsymbol{R}_m)$ by the true Coulomb potential can be justified starting from the wave function (II.12). Substitution of this function into the real expression for $U(\boldsymbol{R}_n - \boldsymbol{R}_m)$ gives

$$U(\boldsymbol{R}_n - \boldsymbol{R}_m) = \sum_{\boldsymbol{q}}\frac{4\pi e^2}{\Omega q^2}e^{-\alpha q^2}e^{i\boldsymbol{q}(\boldsymbol{R}_n - \boldsymbol{R}_m)}$$

$$= \frac{e^2}{|\boldsymbol{R}_n - \boldsymbol{R}_m|}\left[1 - \mathrm{erfc}\left(\frac{|\boldsymbol{R}_n - \boldsymbol{R}_m|}{2\sqrt{\alpha}}\right)\right], \qquad \text{(II.15)}$$

where erfc is the complement of the error function. As $\mathrm{efc}(x) \simeq e^{-x^2}$ for $x \to \infty$, the difference between $U(\boldsymbol{R}_n - \boldsymbol{R}_m)$ and the Coulomb potential is of the order $S(\boldsymbol{R}_n - \boldsymbol{R}_m)^2$, where the overlap $S(\boldsymbol{R}_n - \boldsymbol{R}_m)$ is given in (3.22). Consequently the replacement does not affect $E_H(f)$ provided that all terms of the order of the overlap can be neglected. The minimum of $E_H(f)$ can easily be found by substituting (II.12) into (II.8) and reads:

$$E_H^{(0)} = E_{Cl} + 2N\lambda \ . \tag{II.16}$$

Next we minimize the Hartree-Fock energy up to order $S(\boldsymbol{R}_n - \boldsymbol{R}_m)^2$ starting from the expression

$$E_{HF}(f) = E_H(f) + \Delta E_{HF}(f) \ , \tag{II.17}$$

where $E_H(f)$ and $\Delta E_{HF}(f)$ are given by (II.1) and (I.17) respectively. With the aid of the complete set of harmonic oscillator eigenfunctions $\hat{f}_{\boldsymbol{\jmath}}$ we can express the variational function $\hat{f}$ as

$$\hat{f}(\boldsymbol{k}) = \hat{f}_0(k) + \sum_{\boldsymbol{\jmath} \neq 0} A_{\boldsymbol{\jmath}} \hat{f}_{\boldsymbol{\jmath}}(\boldsymbol{k}) \ , \tag{II.18}$$

where $\hat{f}_0(k)$ is given by (II.12), and the coefficients $A_{\boldsymbol{\jmath}}$ are variational parameters. We remark here that $\hat{f}$ is normalized up to order $S(\boldsymbol{R}_n - \boldsymbol{R}_m)^2$, as will be clear from the following. Substituting (II.18) into (II.17) and using the orthogonality of the functions $\hat{f}_{\boldsymbol{\jmath}}$, $E_{HF}(f)$ can be written in the following form

$$E_{HF}(f) = E_{HF}(f_0) + 2N \sum_{\boldsymbol{\jmath} \neq 0} [C_{\boldsymbol{\jmath}} |A_{\boldsymbol{\jmath}}|^2 - \Delta C_{\boldsymbol{\jmath}} (A_{\boldsymbol{\jmath}} + A_{\boldsymbol{\jmath}}^*)] \ , \tag{II.19}$$

with $E_{HF}(f_0)$ given by (3.27), (3.28) and (3.29), whereas $C_{\boldsymbol{\jmath}}$ and $\Delta C_{\boldsymbol{\jmath}}$ are constants of order $S(\boldsymbol{R}_m - \boldsymbol{R}_n)^0$ and $S(\boldsymbol{R}_m - \boldsymbol{R}_n)^2$ respectively. Minimizing $E_{HF}(f)$ with respect to $A_{\boldsymbol{\jmath}}$ we get

$$A_{\boldsymbol{\jmath}} = \frac{\Delta C_{\boldsymbol{\jmath}}}{C_{\boldsymbol{\jmath}}} \ , \tag{II.20}$$

$$E_{HF}(f) = E_{HF}(f_0) - 2N \sum_{\boldsymbol{\jmath} \neq 0} \frac{\Delta C_{\boldsymbol{\jmath}}^2}{C_{\boldsymbol{\jmath}}} \ . \tag{II.21}$$

Thus the function that minimizes $E_{HF}(f)$ consists of (II.12) and terms of order $S(\boldsymbol{R}_m - \boldsymbol{R}_n)^2$. It follows directly from (II.21) that the contribution of these correction terms to $E_{HF}(f)$ is of order $S(\boldsymbol{R}_m - \boldsymbol{R}_n)^4$. Consequently $E_{HF}(f_0)$ is the correct minimum of $E_{HF}(f)$ up to order $S(\boldsymbol{R}_m - \boldsymbol{R}_n)^2$. The constants $C_{\boldsymbol{J}}$ and $\Delta C_{\boldsymbol{J}}$ can in principle be calculated exactly. In section 3, however, we restrict ourselves to an approximate calculation as the precise form of the wave function seems of little interest.

Appendix III

Consider the following sum over reciprocal lattice vectors

$$E = \sum_{\boldsymbol{K}_n \neq 0} V_\alpha(\boldsymbol{K}_n)\, e^{i\boldsymbol{K}_n \cdot \boldsymbol{a}} , \tag{III.1}$$

where $\boldsymbol{a}$ is an arbitrary vector and the function V_α depends on the variational parameter α as introduced in section 3. After Ewald the parameter β is introduced and E is rewritten as

$$E = \sum_{\boldsymbol{K}_n} [V_\alpha(\boldsymbol{K}_n) - V_\beta(\boldsymbol{K}_n)]\, e^{i\boldsymbol{K}_n \cdot \boldsymbol{a}} - \lim_{\boldsymbol{q}\to 0} [V_\alpha(\boldsymbol{q}) - V_\beta(\boldsymbol{q})] + \sum_{\boldsymbol{K}_n \neq 0} V_\beta(\boldsymbol{K}_n)\, e^{i\boldsymbol{K}_n \cdot \boldsymbol{a}} . \tag{III.2}$$

Next we substitute into (III.2) the Fourier decomposition

$$V_\alpha(\boldsymbol{K}_n) = \frac{1}{\Omega} \int d^3r\, U_\alpha(\boldsymbol{r})\, e^{-i\boldsymbol{K}_n \cdot \boldsymbol{r}} \tag{III.3}$$

with

$$U_\alpha(\boldsymbol{r}) = \sum_{\boldsymbol{q}} V_\alpha(\boldsymbol{q})\, e^{i\boldsymbol{q} \cdot \boldsymbol{r}} = \frac{\Omega}{(2\pi)^3} \int d^3q\, V_\alpha(\boldsymbol{q})\, e^{i\boldsymbol{q} \cdot \boldsymbol{r}} . \tag{III.4}$$

Using the identity

$$\sum_{\boldsymbol{K}_n} e^{-\imath \boldsymbol{K}_n(\boldsymbol{r} - \boldsymbol{a})} = \frac{\Omega}{2N} \sum_{\boldsymbol{R}_n} \delta^3(\boldsymbol{r} - \boldsymbol{a} - \boldsymbol{R}_n) , \tag{III.5}$$

where $\boldsymbol{R}_n$ denotes a lattice vector ($n = 1, 2, \ldots, 2N$), we then obtain

$$E = \frac{1}{2N} \sum_{\boldsymbol{R}_n} [U_\alpha(\boldsymbol{R}_n + \boldsymbol{a}) - U_\beta(\boldsymbol{R}_n + \boldsymbol{a})] - \lim_{\boldsymbol{q}\to 0} [V_\alpha(\boldsymbol{q}) - V_\beta(\boldsymbol{q})] + \sum_{\boldsymbol{K}_n \neq 0} V_\beta(\boldsymbol{K}_n)\, e^{\imath \boldsymbol{K}_n \cdot \boldsymbol{a}} . \tag{III.6}$$

Substitution of (3.24) into (III.6) results into

$$E = \frac{1}{2N} \sum_{\boldsymbol{R}_n} \frac{e^2}{|\boldsymbol{R}_n + \boldsymbol{a}|} \left[\operatorname{erfc}\left(\frac{|\boldsymbol{R}_n + \boldsymbol{a}|}{2\sqrt{\beta}} \right) - \operatorname{erfc}\left(\frac{|\boldsymbol{R}_n + \boldsymbol{a}|}{2\sqrt{\alpha}} \right) \right] + \frac{4\pi e^2}{\Omega} (\alpha - \beta) + \frac{4\pi e^2}{\Omega} \sum_{\boldsymbol{K}_n \neq 0} \frac{e^{-\beta K_n^2}}{K_n^2}\, e^{\imath \boldsymbol{K}_n \cdot \boldsymbol{a}} . \tag{III.7}$$

Putting $\boldsymbol{a} = 0$ the term in (III.7) corresponding with $\boldsymbol{R}_n = 0$ appears to be:

$$\lim_{x \to 0} \frac{e^2}{2N} \left(\frac{[\operatorname{erfc}(x/2\sqrt{\beta}) - \operatorname{erfc}(x/2\sqrt{\alpha})]}{x} \right) = \frac{e^2}{2N} \left(\frac{1}{\sqrt{\pi\alpha}} - \frac{1}{\sqrt{\pi\beta}} \right) . \tag{III.8}$$

Appendix IV

According to Carr [5] the two-particle exchange gives the following contribution to the energy of a ferromagnetic lattice:

$$\Delta E^f_{HF} = -\frac{1}{2}\sum_{i\neq j} J_{ij} \ , \tag{IV.1}$$

where J_{ij} is the two-particle exchange integral

$$\begin{aligned} J_{ij} &= \int d^3r_1 d^3r_2\, f_0^*(\boldsymbol{r}_1 - \boldsymbol{R}_i)\, f_0^*(\boldsymbol{r}_2 - R_j) H(1,2)\, f_0(\boldsymbol{r}_1 - \boldsymbol{R}_j)\, f_0(\boldsymbol{r}_2 - \boldsymbol{R}_i) \\ &- S(\boldsymbol{R}_i - \boldsymbol{R}_j)^2 \int d^3r_1 d^3r_2\, f_0^*(\boldsymbol{r}_1 - \boldsymbol{R}_i)\, f_0^*(\boldsymbol{r}_2 - \boldsymbol{R}_j)\, H(1,2)\, f_0(\boldsymbol{r}_1 - \boldsymbol{R}_i)\, f_0(\boldsymbol{r}_2 - \boldsymbol{R}_j) \ . \end{aligned} \tag{IV.2}$$

The appearing wave function f_0 and the overlap S are given by expressions (3.16) and (3.22), respectively, and the effective two-particle Hamiltonian $H(1,2)$ reads

$$\begin{aligned} H(1,2) &= \frac{-\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - \frac{2N}{\Omega} e^2 \int d^3r \left[\frac{1}{|\boldsymbol{r} - \boldsymbol{r}_1|} + \frac{1}{|\boldsymbol{r} - \boldsymbol{r}_2|}\right] \\ &+ e^2 \sum_{m\neq i,j} \int d^3r\, f_0(\boldsymbol{r} - \boldsymbol{R}_m)^2 \left[\frac{1}{|\boldsymbol{r} - \boldsymbol{r}_1|} + \frac{1}{|\boldsymbol{r} - \boldsymbol{r}_2|}\right] \ . \end{aligned} \tag{IV.3}$$

In order to compare Carr's calculation of the two-particle exchange energy with the present one (IV.3) is substituted into (IV.2) resulting into

$$\begin{aligned} J_{ij} &= e^{-R_{ij}^2/4\alpha} \left\{ \frac{-\hbar^2 R_{ij}^2}{16 m \alpha^2} + \frac{e^2}{\sqrt{\pi\alpha}} - \frac{e^2}{R_{ij}} \operatorname{erf}\left(\frac{R_{ij}}{2\sqrt{\alpha}}\right) \right. \\ &+ \left. 2e^2 \sum_{\boldsymbol{R}_m \neq \boldsymbol{R}_{ij}, 0} \left[\frac{\operatorname{erf}(|\boldsymbol{R}_m - \frac{1}{2}\boldsymbol{R}_{ij}|/2\sqrt{\alpha})}{|\boldsymbol{R}_m - \frac{1}{2}\boldsymbol{R}_{ij}|} - \frac{\operatorname{erf}(R_m/2\sqrt{\alpha})}{R_m} \right] \right\} + \Delta J_{ij}, \end{aligned} \tag{IV.4}$$

where $\boldsymbol{R}_{ij} = \boldsymbol{R}_i - \boldsymbol{R}_j$ and ΔJ_{ij} is the contribution due to the interaction of the electrons with the positive background,

$$\begin{aligned} \Delta J_{ij} &= \int d^3r_1\, d^3r_2\, f_0^*(\boldsymbol{r}_1 - \boldsymbol{R}_i) f_0^*(\boldsymbol{r}_2 - \boldsymbol{R}_j) \Delta H(1,2)\, f_0(\boldsymbol{r}_1 - \boldsymbol{R}_j)\, f_0(\boldsymbol{r}_2 - \boldsymbol{R}_i) \\ &- S(\boldsymbol{R}_i - \boldsymbol{R}_j)^2 \int d^3r_1\, d^3r_2\, f_0^*(\boldsymbol{r}_1 - \boldsymbol{R}_i) f_0^*(\boldsymbol{r}_2 - \boldsymbol{R}_j) \Delta H(1,2)\, f_0(\boldsymbol{r}_1 - \boldsymbol{R}_i)\, f_0(\boldsymbol{r}_2 - \boldsymbol{R}_j) \ , \end{aligned} \tag{IV.5}$$

with

$$\Delta H(1,2) = \frac{-2N}{\Omega}\, e^2 \int d^3r \left[\left(\frac{1}{|\boldsymbol{r} - \boldsymbol{r}_1|} - \frac{1}{r} \right) + \left(\frac{1}{|\boldsymbol{r} - \boldsymbol{r}_2|} - \frac{1}{r} \right) \right] . \qquad \text{(IV.6)}$$

Now the magnitude of ΔJ_{ij} appears to depend on the way the integration in (IV.6) is performed. Carr's procedure consisted of first integrating over a sphere with a given radius L and afterwards taking the limit $L \to \infty$ giving $\Delta H(1,2) = \frac{4\pi N e^2}{3\Omega}(r_1^2 + r_2^2)$ and $\Delta J_{ij} = \frac{-2\pi N e^2}{3\Omega} R_{ij}^2\, e^{-R_{ij}^2/4\alpha}$. This actually means that Carr's definition of the jellium model differs from the usual one as given in section 2. According to the usual definition the Coulomb potential $\frac{1}{r}$ must be replaced by the Yukawa potential $\frac{e^{-\mu r}}{r}$ and the limit $\mu \to 0$ taken after performing the integration. Such a procedure results into $\Delta H(1,2) = \Delta J_{ij} = 0$. Only then the substitution of (IV.4) into (IV.1) leads to the expression (3.28) for the ferromagnetic two-particle exchange energy. That follows directly from the choice $\beta \to \infty$, where β denotes the Ewald parameter. Thus the discrepancy between Carr's and our expression for the exchange energy can be completely understood in terms of two slightly different definitions of the jellium model. This difference in definition, however, does not account for the large discrepancy in critical density for ferromagnetic behaviour. The two critical densities are given by $r_s \simeq 270$ and $r_s \simeq 14$ respectively. Carr's result $r_s \simeq 270$ is based upon the following three approximations for J_{ij}:

(1) The error functions were set equal to one, i.e. J_{ij} was expressed as

$$J_{ij} \simeq e^{-R_{ij}^2/4\alpha} \left\{ -R_{ij}^2 \left[\frac{\hbar^2}{16 m \alpha^2} + \frac{2\pi N e^2}{3\Omega} \right] - \frac{3e^2}{R_{ij}} + \frac{e^2}{\sqrt{\pi \alpha}} + 2e^2 \sum_{\boldsymbol{R}_m \neq 0} \left[|\boldsymbol{R}_m - \frac{1}{2}\boldsymbol{R}_{ij}|^{-1} - R_m^{-1} \right] \right\} . \qquad \text{(IV.7)}$$

(2) The parameter α was given by the Wigner value $\frac{1}{2} r_s^{3/2} a_0^2$.

(3) The contribution of the sum over $\boldsymbol{R}_m$ was neglected in (IV.7).

These approximations lead to a positive nearest neighbour exchange integral, i.e. to a ferromagnetic lattice, for $r_s \simeq 270$. The approximations (1) and (2) are both justified

because they neglect only irrelevant terms, i.e. terms of order $S(\boldsymbol{R}_{ij})^n$, $n \geq 4$. Approximation (3), however, is certainly not justified as follows directly from a calculation of the first few terms in the sum over $\boldsymbol{R}_m$. This is the main reason for the discrepancy between Carr's and the present result. The correct contribution of the sum over $\boldsymbol{R}_m$ can be found using the Ewald summation method, as done in section 3.

Appendix V

The interaction operator V is calculated by substituting (4.37) into (4.30). Then we get up to order q^4:

$$\int d^3k\, \hat{f}_{\jmath}(\boldsymbol{k})\hat{f}^*_{\ell}(\boldsymbol{k}\pm\boldsymbol{q}) =$$

$$e^{-\alpha q^2/2}\prod_{\hat{\boldsymbol{\xi}}}\Big\{\delta_{\jmath\cdot\hat{\boldsymbol{\xi}},\ell\cdot\hat{\boldsymbol{\xi}}} \pm i\sqrt{\alpha}\,\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}}\left[\sqrt{(\jmath\cdot\hat{\boldsymbol{\xi}}+1)}\,\delta_{\jmath\,\hat{\boldsymbol{\xi}}+1,\ell\,\hat{\boldsymbol{\xi}}} + \sqrt{(\ell\cdot\hat{\boldsymbol{\xi}}+1)}\,\delta_{\ell\,\hat{\boldsymbol{\xi}}+1,\jmath\,\hat{\boldsymbol{\xi}}}\right]$$

$$-\alpha(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^2\left[\jmath\cdot\hat{\boldsymbol{\xi}}\,\delta_{\jmath\,\hat{\boldsymbol{\xi}},\ell\,\hat{\boldsymbol{\xi}}} + \frac{1}{2}\sqrt{(\jmath\cdot\hat{\boldsymbol{\xi}}+1)(\jmath\cdot\hat{\boldsymbol{\xi}}+2)}\,\delta_{\jmath\cdot\hat{\boldsymbol{\xi}}+2,\ell\cdot\hat{\boldsymbol{\xi}}}\right.$$

$$\left.+\frac{1}{2}\sqrt{(\ell\cdot\hat{\boldsymbol{\xi}}+1)(\ell\cdot\hat{\boldsymbol{\xi}}+2)}\,\delta_{\ell\cdot\hat{\boldsymbol{\xi}}+2,\jmath\cdot\hat{\boldsymbol{\xi}}}\right] \mp i\alpha\sqrt{\alpha}(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^3\left[\frac{1}{2}(\jmath\cdot\hat{\boldsymbol{\xi}})\sqrt{(\jmath\cdot\hat{\boldsymbol{\xi}}+1)}\,\delta_{\jmath\,\hat{\boldsymbol{\xi}}+1,\ell\,\hat{\boldsymbol{\xi}}}\right.$$

$$+\frac{1}{2}(\ell\cdot\hat{\boldsymbol{\xi}})\sqrt{(\ell\cdot\hat{\boldsymbol{\xi}}+1)}\,\delta_{\ell\cdot\hat{\boldsymbol{\xi}}+1,\jmath\,\hat{\boldsymbol{\xi}}} + \frac{1}{6}\sqrt{(\jmath\cdot\hat{\boldsymbol{\xi}}+1)(\jmath\cdot\hat{\boldsymbol{\xi}}+2)(\jmath\cdot\hat{\boldsymbol{\xi}}+3)}\,\delta_{\jmath\,\hat{\boldsymbol{\xi}}+3,\ell\cdot\hat{\boldsymbol{\xi}}}$$

$$\left.+\frac{1}{6}\sqrt{(\ell\cdot\hat{\boldsymbol{\xi}}+1)(\ell\cdot\hat{\boldsymbol{\xi}}+2)(\ell\cdot\hat{\boldsymbol{\xi}}+3)}\,\delta_{\ell\cdot\hat{\boldsymbol{\xi}}+3,\jmath\,\hat{\boldsymbol{\xi}}}\right]$$

$$+\alpha^2(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^4\left[\frac{1}{6}(\jmath\cdot\hat{\boldsymbol{\xi}})\sqrt{(\jmath\cdot\hat{\boldsymbol{\xi}}+1)(\jmath\cdot\hat{\boldsymbol{\xi}}+2)}\,\delta_{\jmath\cdot\hat{\boldsymbol{\xi}}+2,\ell\cdot\hat{\boldsymbol{\xi}}}\right.$$

$$+\frac{1}{6}(\ell\cdot\hat{\boldsymbol{\xi}})\sqrt{(\ell\cdot\hat{\boldsymbol{\xi}}+1)(\ell\cdot\hat{\boldsymbol{\xi}}+2)}\,\delta_{\ell\,\hat{\boldsymbol{\xi}}+2,\jmath\,\hat{\boldsymbol{\xi}}} + \frac{1}{4}(\jmath\cdot\hat{\boldsymbol{\xi}})(\jmath\cdot\hat{\boldsymbol{\xi}}-1)\delta_{\jmath\,\hat{\boldsymbol{\xi}},\ell\,\hat{\boldsymbol{\xi}}}$$

$$+\frac{1}{24}\sqrt{(\jmath\cdot\hat{\boldsymbol{\xi}}+1)(\jmath\cdot\hat{\boldsymbol{\xi}}+2)(\jmath\cdot\hat{\boldsymbol{\xi}}+3)(\jmath\cdot\hat{\boldsymbol{\xi}}+4)}\,\delta_{\jmath\,\hat{\boldsymbol{\xi}}+4,\ell\cdot\hat{\boldsymbol{\xi}}}$$

$$\left.+\frac{1}{24}\sqrt{(\ell\cdot\hat{\boldsymbol{\xi}}+1)(\ell\cdot\hat{\boldsymbol{\xi}}+2)(\ell\cdot\hat{\boldsymbol{\xi}}+3)(\ell\cdot\hat{\boldsymbol{\xi}}+4)}\,\delta_{\ell\,\hat{\boldsymbol{\xi}}+4,\jmath\,\hat{\boldsymbol{\xi}}}\right] \tag{V.1}$$

and

$$\sum_{\jmath,\ell}\int d^3k\,\hat{f}_{\jmath}(\boldsymbol{k})\,\hat{f}^*_{\ell}(\boldsymbol{k}\pm\boldsymbol{q})\,D^n_{\jmath\ell} =$$

$$
\begin{aligned}
& e^{-\frac{1}{2}\alpha q^2}\left\{ S^n_{\mathbf{0}} + \sum_{\hat{\boldsymbol{\xi}}}\left[\pm i\sqrt{\alpha}\,(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})\, S^n_{\hat{\boldsymbol{\xi}}} - \alpha(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^2\, S^n_{2\hat{\boldsymbol{\xi}}} \right.\right. \\
& \left. + \mp\, i\alpha\sqrt{\alpha}\,(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^3\, S^n_{3\hat{\boldsymbol{\xi}}} + \alpha^2(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^4\, S^n_{4\hat{\boldsymbol{\xi}}} \right] \\
& + \sum_{\hat{\boldsymbol{\xi}}\neq\hat{\boldsymbol{\eta}}}\left[-\frac{1}{2}\,\alpha(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})(\boldsymbol{q}\cdot\hat{\boldsymbol{\eta}})\, S^n_{\hat{\boldsymbol{\xi}}+\hat{\boldsymbol{\eta}}} \mp i\alpha\sqrt{\alpha}\,(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^2(\boldsymbol{q}\cdot\hat{\boldsymbol{\eta}})\, S^n_{2\hat{\boldsymbol{\xi}}+\hat{\boldsymbol{\eta}}} \right. \\
& \left. + \frac{1}{2}\,\alpha^2(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^2(\boldsymbol{q}\cdot\hat{\boldsymbol{\eta}})^2\, S^n_{2\hat{\boldsymbol{\xi}}+2\hat{\boldsymbol{\eta}}} + \alpha^2(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^3(\boldsymbol{q}\cdot\hat{\boldsymbol{\eta}})\, S^n_{3\hat{\boldsymbol{\xi}}+\hat{\boldsymbol{\eta}}} \right] \\
& + \sum_{\hat{\boldsymbol{\zeta}}\neq\hat{\boldsymbol{\xi}}\neq\hat{\boldsymbol{\eta}}\neq\hat{\boldsymbol{\zeta}}}\left[\mp\frac{1}{6}\, i\alpha\sqrt{\alpha}\,(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})(\boldsymbol{q}\cdot\hat{\boldsymbol{\eta}})(\boldsymbol{q}\cdot\boldsymbol{\zeta})\, S^n_{\hat{\boldsymbol{\xi}}+\hat{\boldsymbol{\eta}}+\hat{\boldsymbol{\zeta}}} \right. \\
& \left.\left. + \frac{1}{2}\,\alpha^2(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^2(\boldsymbol{q}\cdot\hat{\boldsymbol{\eta}})(\boldsymbol{q}\cdot\hat{\boldsymbol{\zeta}})\, S^n_{2\hat{\boldsymbol{\xi}}+\hat{\boldsymbol{\eta}}+\hat{\boldsymbol{\zeta}}} \right] \right\} \qquad \text{(V.2)}
\end{aligned}
$$

with

$$
\begin{aligned}
S^n_{\mathbf{0}} &= \sum_{\boldsymbol{\jmath}} D^n_{\boldsymbol{\jmath}\boldsymbol{\jmath}}\,, \\
S^n_{\hat{\boldsymbol{\xi}}} &= \sum_{\boldsymbol{\jmath}} \sqrt{(\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}+1)}\,\left[D^n_{\boldsymbol{\jmath},\boldsymbol{\jmath}+\hat{\boldsymbol{\xi}}} + D^n_{\boldsymbol{\jmath}+\hat{\boldsymbol{\xi}},\boldsymbol{\jmath}} \right]\,, \\
S^n_{2\hat{\boldsymbol{\xi}}} &= \sum_{\boldsymbol{\jmath}} \left[(\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}})\, D^n_{\boldsymbol{\jmath}\boldsymbol{\jmath}} + \frac{1}{2}\sqrt{(\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}+1)(\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}+2)}\,\left[D^n_{\boldsymbol{\jmath},\boldsymbol{\jmath}+2\hat{\boldsymbol{\xi}}} + D^n_{\boldsymbol{\jmath}+2\hat{\boldsymbol{\xi}},\boldsymbol{\jmath}} \right] \right]\,, \\
S^n_{3\hat{\boldsymbol{\xi}}} &= \sum_{\boldsymbol{\jmath}} \left[\frac{1}{2}\sqrt{(\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}+1)}\left[D^n_{\boldsymbol{\jmath},\boldsymbol{\jmath}+\hat{\boldsymbol{\xi}}} + D^n_{\boldsymbol{\jmath}+\hat{\boldsymbol{\xi}},\boldsymbol{\jmath}} \right] \right. \\
&\quad + \left. \frac{1}{6}\sqrt{(\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}+1)(\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}+2)(\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}+3)}\,\left[D^n_{\boldsymbol{\jmath},\boldsymbol{\jmath}+3\hat{\boldsymbol{\xi}}} + D^n_{\boldsymbol{\jmath}+3\hat{\boldsymbol{\xi}},\boldsymbol{\jmath}} \right] \right]\,, \\
S^n_{4\hat{\boldsymbol{\xi}}} &= \sum_{\boldsymbol{\jmath}} \left[\frac{1}{4}\,\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}(\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}-1) D^n_{\boldsymbol{\jmath}\boldsymbol{\jmath}} + \frac{1}{6}\,(\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}})\sqrt{(\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}+1)(\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}+2)}\,\left[D^n_{\boldsymbol{\jmath},\boldsymbol{\jmath}+2\hat{\boldsymbol{\xi}}} + D^n_{\boldsymbol{\jmath}+2\hat{\boldsymbol{\xi}},\boldsymbol{\jmath}} \right] \right. \\
&\quad + \left. \frac{1}{24}\sqrt{(\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}+1)(\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}+2)(\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}+3)(\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}+4)}\,\left[D^n_{\boldsymbol{\jmath},\boldsymbol{\jmath}+4\hat{\boldsymbol{\xi}}} + D^n_{\boldsymbol{\jmath}+4\hat{\boldsymbol{\xi}},\boldsymbol{\jmath}} \right] \right]\,, \\
S^n_{\hat{\boldsymbol{\xi}}+\hat{\boldsymbol{\eta}}} &= \sum_{\boldsymbol{\jmath}} \sqrt{(\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}+1)(\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\eta}}+1)}\,\left[D^n_{\boldsymbol{\jmath},\boldsymbol{\jmath}+\hat{\boldsymbol{\xi}}+\hat{\boldsymbol{\eta}}} + D^n_{\boldsymbol{\jmath}+\boldsymbol{\eta},\boldsymbol{\jmath}+\hat{\boldsymbol{\xi}}} + D^n_{\boldsymbol{\jmath}+\hat{\boldsymbol{\xi}},\boldsymbol{\jmath}+\hat{\boldsymbol{\eta}}} + D^n_{\boldsymbol{\jmath}+\hat{\boldsymbol{\xi}}+\hat{\boldsymbol{\eta}},\boldsymbol{\jmath}} \right]\,, \\
S^n_{2\hat{\boldsymbol{\xi}}+\hat{\boldsymbol{\eta}}} &= \sum_{\boldsymbol{\jmath}} \left[\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}\sqrt{(\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\eta}}+1)}\,\left[D^n_{\boldsymbol{\jmath},\boldsymbol{\jmath}+\hat{\boldsymbol{\eta}}} + D_{\boldsymbol{\jmath}+\hat{\boldsymbol{\eta}},\boldsymbol{\jmath}} \right] \right. \\
&\quad + \left. \frac{1}{2}\sqrt{(\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\eta}}+1)(\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}+1)(\boldsymbol{\jmath}\cdot\hat{\boldsymbol{\xi}}+2)}\,\left[D^n_{\boldsymbol{\jmath},\boldsymbol{\jmath}+2\hat{\boldsymbol{\xi}}+\hat{\boldsymbol{\eta}}} + D^n_{\boldsymbol{\jmath}+\hat{\boldsymbol{\eta}},\boldsymbol{\jmath}+2\hat{\boldsymbol{\xi}}} \right.\right.
\end{aligned}
$$

$$
\begin{aligned}
&+ \quad D^n_{\jmath+2\hat{\xi},\jmath+\hat{\eta}} + D^n_{\jmath+2\hat{\xi}+\hat{\eta},\jmath}\Big]\Big] \ , \\
S^n_{2\hat{\xi}+2\hat{\eta}} &= \sum_{\jmath}\Big[(\jmath\cdot\hat{\xi})(\jmath\cdot\hat{\eta})D^n_{\jmath\jmath} + \frac{1}{2}\jmath\cdot\hat{\xi}\sqrt{(\jmath\cdot\hat{\eta}+1)(\jmath\cdot\hat{\eta}+2)}\,\Big[D^n_{\jmath,\jmath+2\hat{\eta}} + D^n_{\jmath+2\hat{\eta},\jmath}\Big] \\
&+ \quad \frac{1}{2}\jmath\cdot\hat{\eta}\sqrt{(\jmath\cdot\hat{\xi}+1)(\jmath\cdot\hat{\xi}+2)}\,\Big[D^n_{\jmath,\jmath+2\hat{\xi}} + D^n_{\jmath+2\hat{\xi},\jmath}\Big] \\
&+ \quad \frac{1}{4}\sqrt{(\jmath\cdot\hat{\xi}+1)(\jmath\cdot\hat{\xi}+2)(\jmath\cdot\hat{\eta}+1)(\jmath\cdot\hat{\eta}+2)}\,\Big[D^n_{\jmath,\jmath+2\hat{\eta}+2\hat{\xi}} + D^n_{\jmath+2\hat{\eta},\jmath+2\hat{\xi}} \\
&+ \quad D^n_{\jmath+2\hat{\xi},\jmath+2\hat{\eta}} + D^n_{\jmath+2\hat{\eta}+2\hat{\xi},\jmath}\Big]\Big] \ , \\
S^n_{3\hat{\xi}+\hat{\eta}} &= \sum_{\jmath}\Big[\frac{1}{2}\jmath\cdot\hat{\xi}\sqrt{(\jmath\cdot\hat{\xi}+1)(\jmath\cdot\hat{\eta}+1)}\,\Big[D^n_{\jmath,\jmath+\hat{\xi}+\hat{\eta}} + D^n_{\jmath+\hat{\xi},\jmath+\hat{\eta}} + D^n_{\jmath+\hat{\eta},\jmath+\hat{\xi}} \\
&+ \quad D^n_{\jmath+\hat{\xi}+\hat{\eta},\jmath}\Big] + \frac{1}{6}\sqrt{(\jmath\cdot\hat{\xi}+1)(\jmath\cdot\hat{\xi}+2)(\jmath\cdot\hat{\xi}+3)(\jmath\cdot\hat{\eta}+1)}\,\Big[D^n_{\jmath,\jmath+3\hat{\xi}+\hat{\eta}} \\
&+ \quad D^n_{\jmath+\hat{\eta},\jmath+3\hat{\xi}} + D^n_{\jmath+3\hat{\xi},\jmath+\hat{\eta}} + D^n_{\jmath+3\hat{\xi}+\hat{\eta},\jmath}\Big]\Big] \ , \\
S^n_{\hat{\xi}+\hat{\eta}+\hat{\zeta}} &= \sum_{\jmath}\sqrt{(\jmath\cdot\hat{\xi}+1)(\jmath\cdot\hat{\eta}+1)(\jmath\cdot\hat{\zeta}+1)}\,\Big[D^n_{\jmath,\jmath+\hat{\xi}+\hat{\eta}+\hat{\zeta}} + D^n_{\jmath+\zeta,\jmath+\hat{\xi}+\hat{\eta}} \\
&+ \quad D^n_{\jmath+\hat{\xi}+\hat{\eta},\jmath+\hat{\zeta}} + D^n_{\jmath+\hat{\xi}+\hat{\eta}+\hat{\zeta},\jmath} + D^n_{\jmath+\eta,\jmath+\hat{\xi}+\hat{\zeta}} + D^n_{\jmath+\hat{\xi}+\hat{\zeta},\jmath+\hat{\eta}} \\
&+ \quad D^n_{\jmath+\hat{\xi},\jmath+\hat{\eta}+\hat{\zeta}} + D^n_{\jmath+\hat{\eta}+\hat{\zeta},\jmath+\hat{\xi}}\Big] \ , \\
S^n_{2\hat{\xi}+\hat{\eta}+\hat{\zeta}} &= \sum_{\jmath}\Big[\jmath\cdot\hat{\xi}\sqrt{(\jmath\cdot\hat{\eta}+1)(\jmath\cdot\hat{\zeta}+1)}\,\Big[D^n_{\jmath,\jmath+\hat{\eta}+\hat{\zeta}} + D^n_{\jmath+\eta,\jmath+\hat{\zeta}} + D^n_{\jmath+\hat{\zeta},\jmath+\hat{\eta}} \\
&+ \quad D^n_{\jmath+\hat{\eta}+\hat{\zeta},\jmath}\Big] + \frac{1}{2}\sqrt{(\jmath\cdot\hat{\xi}+1)(\jmath\cdot\hat{\xi}+2)(\jmath\cdot\hat{\eta}+1)(\jmath\cdot\hat{\zeta}+1)}\,\Big[D^n_{\jmath,\jmath+2\hat{\xi}+\hat{\eta}+\hat{\zeta}} \\
&+ \quad D^n_{\jmath+\zeta,\jmath+2\hat{\xi}+\hat{\eta}} + D^n_{\jmath+2\hat{\xi}+\jmath+\hat{\eta}+\hat{\zeta}} + D^n_{\jmath+2\hat{\xi}+\hat{\zeta},\jmath+\hat{\eta}} + D^n_{\jmath+\eta,\jmath+2\hat{\xi}+\hat{\zeta}} \\
&+ \quad D^n_{\jmath+\hat{\eta}+\hat{\zeta},\jmath+2\hat{\xi}} + D^n_{\jmath+2\hat{\xi}+\hat{\eta},\jmath+\hat{\zeta}} + D^n_{\jmath+\hat{\eta}+2\hat{\xi}+\hat{\zeta},\jmath}\Big]\Big] \ . \qquad \text{(V.3)}
\end{aligned}
$$

Using the effective properties (4.34) and (4.35) of the operators $D^n_{\jmath_1\jmath_2}$ the following expressions for the operators as defined in (V.3) are obtained:

$$
S^n_{\mathbf{0}} \ = \ 1 \ , \quad S^n_{2\hat{\xi}} = \frac{1}{2}S^n_{\hat{\xi}}S^n_{\hat{\xi}} - \frac{1}{2} \ ,
$$

$$
S^n_{3\hat{\xi}} \ = \ \frac{1}{6}S^n_{\hat{\xi}}S^n_{\hat{\xi}}S^n_{\hat{\xi}} - \frac{1}{2}S^n_{\hat{\xi}} \ ,
$$

$$S^n_{4\hat{\boldsymbol{\xi}}} = \frac{1}{24} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} - \frac{1}{4} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} + \frac{1}{8} ,$$

$$S^n_{\hat{\boldsymbol{\xi}}+\hat{\boldsymbol{\eta}}} = S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} , \quad S^n_{2\hat{\boldsymbol{\xi}}+\hat{\boldsymbol{\eta}}} = \frac{1}{2} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} - \frac{1}{2} S^n_{\hat{\boldsymbol{\eta}}} ,$$

$$S^n_{2\hat{\boldsymbol{\xi}}+2\hat{\boldsymbol{\eta}}} = \frac{1}{4} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} S^n_{\hat{\boldsymbol{\eta}}} - \frac{1}{4} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} - \frac{1}{4} S^n_{\hat{\boldsymbol{\eta}}} S^n_{\hat{\boldsymbol{\eta}}} + \frac{1}{4} ,$$

$$S^n_{3\hat{\boldsymbol{\xi}}+\hat{\boldsymbol{\eta}}} = \frac{1}{6} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} - \frac{1}{2} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} ,$$

$$S^n_{\hat{\boldsymbol{\xi}}+\hat{\boldsymbol{\eta}}+\hat{\boldsymbol{\zeta}}} = S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} S^n_{\hat{\boldsymbol{\zeta}}} , \quad S^n_{2\hat{\boldsymbol{\xi}}+\hat{\boldsymbol{\eta}}+\hat{\boldsymbol{\zeta}}} = \frac{1}{2} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} S^n_{\hat{\boldsymbol{\zeta}}} - \frac{1}{2} S^n_{\hat{\boldsymbol{\eta}}} S^n_{\hat{\boldsymbol{\zeta}}} . \qquad \text{(V.4)}$$

Substituting (V.4) into (V.2) we arrive at:

$$\begin{aligned}
&\sum_{\jmath,\boldsymbol{\ell}} \int d^3k\, \hat{f}_{\jmath}(\boldsymbol{k})\, \hat{f}^*_{\boldsymbol{\ell}}(\boldsymbol{k} \pm \boldsymbol{q})\, D^n_{\jmath\boldsymbol{\ell}} \\
&= e^{-\frac{1}{2}\alpha q^2} \left\{ 1 + \sum_{\hat{\boldsymbol{\xi}}} \left[\pm i\sqrt{\alpha}\, (\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})\, S^n_{\hat{\boldsymbol{\xi}}} - \alpha(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^2 \left[\frac{1}{2} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} - \frac{1}{2} \right] \right.\right. \\
&+ \left.\left. \mp i\alpha\sqrt{\alpha}\,(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^3 \left[\frac{1}{6} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} - \frac{1}{2} S^n_{\hat{\boldsymbol{\xi}}} \right] + \alpha^2 (\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^4 \left[\frac{1}{24} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} - \frac{1}{4} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} + \frac{1}{8} \right] \right] \\
&+ \sum_{\hat{\boldsymbol{\xi}}\neq\hat{\boldsymbol{\eta}}} \left[-\frac{1}{2} \alpha(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})(\boldsymbol{q}\cdot\hat{\boldsymbol{\eta}}) \left[S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} \right] \mp i\alpha\sqrt{\alpha}\,(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^2 (\boldsymbol{q}\cdot\hat{\boldsymbol{\eta}}) \left[\frac{1}{2} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} - \frac{1}{2} S^n_{\hat{\boldsymbol{\eta}}} \right] \right. \\
&+ \frac{1}{2} \alpha^2 (\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^2 (\boldsymbol{q}\cdot\hat{\boldsymbol{\eta}})^2 \left[\frac{1}{4} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} S^n_{\hat{\boldsymbol{\eta}}} - \frac{1}{4} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} - \frac{1}{4} S^n_{\hat{\boldsymbol{\eta}}} S^n_{\hat{\boldsymbol{\eta}}} + \frac{1}{4} \right] \\
&+ \left. \alpha^2 (\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^3 (\boldsymbol{q}\cdot\hat{\boldsymbol{\eta}}) \left[\frac{1}{6} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} - \frac{1}{2} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} \right] \right] \\
&+ \sum_{\hat{\boldsymbol{\zeta}}\neq\hat{\boldsymbol{\xi}}\neq\hat{\boldsymbol{\eta}}\neq\hat{\boldsymbol{\zeta}}} \left[\mp \frac{1}{6} i\alpha\sqrt{\alpha} (\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})(\boldsymbol{q}\cdot\hat{\boldsymbol{\eta}})(\boldsymbol{q}\cdot\hat{\boldsymbol{\zeta}})\, S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} S^n_{\hat{\boldsymbol{\zeta}}} \right. \\
&+ \left. \left. \frac{1}{2} \alpha^2 (\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^2 (\boldsymbol{q}\cdot\hat{\boldsymbol{\eta}})(\boldsymbol{q}\cdot\hat{\boldsymbol{\zeta}}) \left[\frac{1}{2} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} S^n_{\hat{\boldsymbol{\zeta}}} - \frac{1}{2} S^n_{\hat{\boldsymbol{\eta}}} S^n_{\hat{\boldsymbol{\zeta}}} \right] \right] \right\} . \qquad \text{(V.5)}
\end{aligned}$$

Now the interaction operator V is given by

$$
\begin{aligned}
V \equiv & \sum_{\jmath_1\jmath_2\ell_1\ell_2} \frac{1}{2} \sum_{n\neq m} e^{i\boldsymbol{q}\cdot\boldsymbol{R}_{nm}} \frac{4\pi e^2}{\Omega q^2} \int d^3k\, d^3k'\, \hat{f}_{\jmath_1}(\boldsymbol{k}) \hat{f}_{\jmath_2}(\boldsymbol{k}') \hat{f}^*_{\ell_2}(\boldsymbol{k}'+\boldsymbol{q}) \hat{f}^*_{\ell_1}(\boldsymbol{k}-\boldsymbol{q}) D^n_{\jmath_1\ell_1} D^m_{\jmath_2\ell_2} \\
= & \frac{1}{2} \sum_{n\neq m} e^{i\boldsymbol{q}\cdot\boldsymbol{R}_{nm}} \frac{4\pi e^2}{\Omega q^2} e^{-\alpha q^2} \left\{ 1 + \sum_{\hat{\boldsymbol{\xi}}} \left[-i\sqrt{\alpha}(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}}) \left[S^n_{\hat{\boldsymbol{\xi}}} - S^m_{\hat{\boldsymbol{\xi}}} \right] \right. \right. \\
- & \alpha(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^2 \left[\frac{1}{2} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} + \frac{1}{2} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} - 1 - S^n_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} \right] + i\alpha\sqrt{\alpha}(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^3 \left[\frac{1}{6} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} \right. \\
- & S^n_{\hat{\boldsymbol{\xi}}} - \frac{1}{6} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} + S^m_{\hat{\boldsymbol{\xi}}} + \frac{1}{2} S^n_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} - \frac{1}{2} S^m_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} \left. \right] + \alpha^2(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^4 \left[\frac{1}{24} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} \right. \\
+ & \frac{1}{24} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} - \frac{1}{2} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} - \frac{1}{2} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} + \frac{1}{2} + \frac{1}{4} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} - \frac{1}{6} S^n_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} \\
+ & \left. \left. S^n_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} - \frac{1}{6} S^m_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} \right] \right] + \sum_{\hat{\boldsymbol{\xi}}\neq\hat{\boldsymbol{\eta}}} \left[-\alpha(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})(\boldsymbol{q}\cdot\hat{\boldsymbol{\eta}}) \left[\frac{1}{2} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} + \frac{1}{2} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\eta}}} - S^n_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\eta}}} \right] \right. \\
+ & i\alpha\sqrt{\alpha}(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^2(\boldsymbol{q}\cdot\hat{\boldsymbol{\eta}}) \left[\frac{1}{2} S^n_{\hat{\boldsymbol{\eta}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} - S^n_{\hat{\boldsymbol{\eta}}} - \frac{1}{2} S^m_{\hat{\boldsymbol{\eta}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} + S^m_{\hat{\boldsymbol{\eta}}} + \frac{1}{2} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} \right. \\
- & \frac{1}{2} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\eta}}} + S^n_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\eta}}} - S^m_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} + S^n_{\hat{\boldsymbol{\eta}}} \left. \right] + \alpha^2(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^2(\boldsymbol{q}\cdot\hat{\boldsymbol{\eta}})^2 \left[\frac{1}{4} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\eta}}} S^m_{\hat{\boldsymbol{\eta}}} \right. \\
- & \frac{1}{2} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} - \frac{1}{2} S^m_{\hat{\boldsymbol{\eta}}} S^m_{\hat{\boldsymbol{\eta}}} + \frac{1}{2} - \frac{1}{2} S^n_{\hat{\boldsymbol{\eta}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\eta}}} + S^n_{\hat{\boldsymbol{\eta}}} S^m_{\hat{\boldsymbol{\eta}}} - \frac{1}{2} S^m_{\hat{\boldsymbol{\eta}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} + \frac{1}{2} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\eta}}} \\
+ & \left. \left. \frac{1}{8} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} S^n_{\hat{\boldsymbol{\eta}}} + \frac{1}{8} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\eta}}} S^m_{\hat{\boldsymbol{\eta}}} \right] + \alpha^2(\boldsymbol{q}\cdot\hat{\boldsymbol{\xi}})^3(\boldsymbol{q}\cdot\hat{\boldsymbol{\eta}}) \left[-\frac{1}{6} S^n_{\hat{\boldsymbol{\eta}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} + \frac{1}{2} S^n_{\hat{\boldsymbol{\eta}}} S^m_{\hat{\boldsymbol{\xi}}} \right.
\end{aligned}
$$

$$
\begin{aligned}
&- \frac{1}{6} S^m_{\hat{\boldsymbol{\eta}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} + \frac{1}{2} S^m_{\hat{\boldsymbol{\eta}}} S^n_{\hat{\boldsymbol{\xi}}} - \frac{1}{2} S^n_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\eta}}} + \frac{1}{2} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\eta}}} - \frac{1}{2} S^m_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} + \frac{1}{2} S^m_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} \\
&+ \frac{1}{2} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\eta}}} - S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\eta}}} + \frac{1}{2} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} - S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} + \frac{1}{6} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} \\
&+ \frac{1}{6} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\eta}}} \Big] \Big] + \sum_{\hat{\boldsymbol{\zeta}} \neq \hat{\boldsymbol{\xi}} \neq \hat{\boldsymbol{\eta}} \neq \hat{\boldsymbol{\zeta}}} \Big[i\alpha^2 \sqrt{\alpha} (\boldsymbol{q} \cdot \hat{\boldsymbol{\xi}})(\boldsymbol{q} \cdot \hat{\boldsymbol{\eta}})(\boldsymbol{q} \cdot \hat{\boldsymbol{\zeta}}) \\
&\times \left[\frac{1}{2} S^n_{\hat{\boldsymbol{\zeta}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\eta}}} - \frac{1}{2} S^m_{\hat{\boldsymbol{\zeta}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} + \frac{1}{6} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} S^n_{\hat{\boldsymbol{\zeta}}} - \frac{1}{6} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\eta}}} S^m_{\hat{\boldsymbol{\zeta}}} \right] \\
&+ \alpha^2 (\boldsymbol{q} \cdot \hat{\boldsymbol{\xi}})^2 (\boldsymbol{q} \cdot \hat{\boldsymbol{\eta}})(\boldsymbol{q} \cdot \hat{\boldsymbol{\zeta}}) \left[\frac{1}{4} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} S^n_{\hat{\boldsymbol{\zeta}}} + \frac{1}{4} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\eta}}} S^m_{\hat{\boldsymbol{\zeta}}} - \frac{1}{2} S^n_{\hat{\boldsymbol{\eta}}} S^n_{\hat{\boldsymbol{\zeta}}} - \frac{1}{2} S^m_{\hat{\boldsymbol{\eta}}} S^m_{\hat{\boldsymbol{\zeta}}} \right. \\
&- \frac{1}{2} S^n_{\hat{\boldsymbol{\zeta}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\eta}}} + S^n_{\hat{\boldsymbol{\zeta}}} S^m_{\hat{\boldsymbol{\eta}}} - \frac{1}{2} S^m_{\hat{\boldsymbol{\zeta}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} - \frac{1}{2} S^n_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\eta}}} S^m_{\hat{\boldsymbol{\zeta}}} - \frac{1}{2} S^m_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} S^n_{\hat{\boldsymbol{\zeta}}} \\
&+ \left. \frac{1}{4} S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\zeta}}} S^m_{\hat{\boldsymbol{\eta}}} + \frac{1}{4} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\zeta}}} S^n_{\hat{\boldsymbol{\eta}}} + S^n_{\hat{\boldsymbol{\xi}}} S^n_{\hat{\boldsymbol{\eta}}} S^m_{\hat{\boldsymbol{\xi}}} S^m_{\hat{\boldsymbol{\zeta}}} \right] \Big] \Big\} \,, \qquad \text{(V.6)}
\end{aligned}
$$

where all terms containing q^M, $M > 4$, have been neglected. In terms of the operators $\boldsymbol{S}_n$, given by (4.39), we can express the interaction operator up to order q^4 as

$$
\begin{aligned}
V \;=\; & \frac{1}{2} \sum_{n \neq m} {\sum_{\boldsymbol{q}}}' e^{i\boldsymbol{q} \cdot \boldsymbol{R}_{nm}} \frac{4\pi e^2}{\Omega q^2} e^{-\alpha q^2} \Big\{ 1 + \sqrt{\alpha} \left[i\boldsymbol{q} \cdot (\boldsymbol{S}_m - \boldsymbol{S}_n) \right] \\
&+ \frac{1}{2} \alpha \left[i\boldsymbol{q} \cdot (\boldsymbol{S}_m - \boldsymbol{S}_n) \right]^2 + \frac{1}{6} \alpha \sqrt{\alpha} \left[i\boldsymbol{q} \cdot (\boldsymbol{S}_m - \boldsymbol{S}_n) \right]^3 + \frac{1}{24} \alpha^2 \left[i\boldsymbol{q} \cdot (\boldsymbol{S}_m - \boldsymbol{S}_n) \right]^4 \\
&+ \alpha q^2 + \alpha \sqrt{\alpha} \left[i\boldsymbol{q} \cdot (\boldsymbol{S}_m - \boldsymbol{S}_n] \, q^2 + \frac{1}{2} \alpha^2 \left[q^2 + \left[i\boldsymbol{q} \cdot (\boldsymbol{S}_m - \boldsymbol{S}_n) \right]^2 \right] q^2 \Big\} \qquad \text{(V.7)}
\end{aligned}
$$

with

$$\frac{1}{2}\sum_{n\neq m}\sum_{\boldsymbol{q}}{}' e^{\imath\boldsymbol{q}\cdot\boldsymbol{R}_{nm}}\frac{4\pi e^2}{\Omega q^2}e^{-\alpha q^2} = E_{Cl} + 2N\left[\frac{4\pi N e^2\alpha}{\Omega} - \frac{1}{2}e^2\sum_{n\neq 0}\frac{1}{R_n}\,\mathrm{erfc}\left(\frac{R_n}{2\sqrt{\alpha}}\right)\right],$$

$$\frac{1}{2}\sum_{n\neq m}\sum_{\boldsymbol{q}}{}' e^{\imath\boldsymbol{q}\cdot\boldsymbol{R}_{nm}}\frac{4\pi e^2}{\Omega}e^{-\alpha q^2} = 2N\left[\frac{-4\pi N e^2}{\Omega} + \sum_{n\neq 0}\frac{e^2}{4\alpha\sqrt{\pi\alpha}}e^{-R_n^2/4\alpha}\right],$$

$$\frac{1}{2}\sum_{n\neq m}\sum_{\boldsymbol{q}}{}' e^{\imath\boldsymbol{q}\cdot\boldsymbol{R}_{nm}}\frac{4\pi e^2}{\Omega}q^2 e^{-\alpha q^2} = 2N\sum_{n\neq 0}\frac{e^2}{16\alpha^3\sqrt{\pi\alpha}}(6\alpha - R_n^2)\,e^{-R_n^2/4\alpha},$$

$$\frac{1}{2}\sum_{n\neq m}\sum_{\boldsymbol{q}}{}' e^{\imath\boldsymbol{q}\cdot\boldsymbol{R}_{nm}}\frac{4\pi e^2}{\Omega}\left[\boldsymbol{q}\cdot(\boldsymbol{S}_n - \boldsymbol{S}_m)\right]^2 e^{-\alpha q^2} =$$

$$2N\sum_{n\neq 0}\frac{e^2}{16\alpha^3\sqrt{\pi\alpha}}\left(5|\boldsymbol{S}_n - \boldsymbol{S}_m|^2\alpha - \frac{1}{2}R_n^2|\boldsymbol{S}_n - \boldsymbol{S}_m|^2 - [\boldsymbol{R}_n\cdot(\boldsymbol{S}_n - \boldsymbol{S}_m)]^2\right)e^{-R_n^2/4\alpha} \tag{V.8}$$

and

$$\frac{1}{2}\sum_{n\neq m}\sum_{\boldsymbol{q}}{}' e^{\imath\boldsymbol{q}\cdot\boldsymbol{R}_{nm}}\frac{4\pi e^2}{\Omega q^2}e^{-\alpha q^2}\begin{cases}[\sqrt{\alpha}\,\imath\boldsymbol{q}\cdot(\boldsymbol{S}_m - \boldsymbol{S}_n)] &= 0\\ \\ \alpha\sqrt{\alpha}\,[\imath\boldsymbol{q}\cdot(\boldsymbol{S}_m - \boldsymbol{S}_n)]\,q^2 &= 0\end{cases}, \tag{V.9}$$

where use is made of the cubic symmetry of the lattice in calculating (V.9). Substitution of (V.8) and (V.9) into (V.7) leads to expression (4.38), where we have neglected all terms containing $\exp[-R_n^2/4\alpha]$ and $\mathrm{erfc}\left(\frac{R_n}{2\sqrt{\alpha}}\right)$.

Higher order contributions to V, i.e. contributions containing $(\boldsymbol{S}_m - \boldsymbol{S}_n)^M$, $M > 4$, can be found analogously and are expected to be given by the following expression, that holds also for $M = 3$ and $M = 4$:

$$\begin{aligned}V_M &= \frac{1}{2}\sum_{n\neq m}\sum_{\boldsymbol{q}}{}' e^{\imath\boldsymbol{q}\cdot\boldsymbol{R}_{nm}}\frac{4\pi e^2}{\Omega q^2}e^{-\alpha q^2}\left[\frac{1}{M!}\alpha^{\frac{1}{2}M}[\imath\boldsymbol{q}\ \ (\boldsymbol{S}_m - \boldsymbol{S}_n)]^M\right]\\ &= \frac{1}{2}\sum_{n\neq m}\left[\frac{1}{M!}\alpha^{\frac{1}{2}M}[(\boldsymbol{S}_m - \boldsymbol{S}_n)\cdot\boldsymbol{\nabla}_{nm}]^M\right]\left(\frac{e^2}{R_{nm}}\right),\end{aligned} \tag{V.10}$$

where all terms of the order of the overlap are neglected, and the gradient operator $\boldsymbol{\nabla}_{nm}$ is given by

$$\boldsymbol{\nabla}_{nm} = \sum_{\hat{\boldsymbol{\xi}}}\hat{\boldsymbol{\xi}}\frac{\partial}{\partial(\boldsymbol{R}_{nm}\cdot\hat{\boldsymbol{\xi}})}. \tag{V.11}$$

Using the results of section 4 the effective Hamiltonian can be written as

$$H_{\text{eff}} = E_{CI} + \sum_{\boldsymbol{k}\lambda} \left(\frac{1}{2} + A^{+}_{\boldsymbol{k}\lambda} A_{\boldsymbol{k}\lambda} \right) \hbar\omega_{\boldsymbol{k}\lambda} + \sum_{M=3}^{\infty} V_M \ , \tag{V.12}$$

where the boson operators $A^{(+)}_{\boldsymbol{k}\lambda}$ are related with the operators $\boldsymbol{S}_n$ according to

$$\boldsymbol{S}_n = \frac{1}{\sqrt{2N}} \sum_{\boldsymbol{k}\lambda} \sqrt{\frac{\hbar}{2m\alpha\omega_{\boldsymbol{k}\lambda}}}\, e^{i\boldsymbol{k}\cdot\boldsymbol{R}_n}\, \boldsymbol{\epsilon}_{\boldsymbol{k}\lambda} [A^{+}_{\boldsymbol{k}\lambda} + A_{\boldsymbol{k}\lambda}] \ . \tag{V.13}$$

Substituting (V.13) into (V.10) we find that the contribution of V_M to the effective Hamiltonian consists of terms proportional to $R_{mn}^{-M-1}\, \omega_{\boldsymbol{k}\lambda}^{-\frac{1}{2}M}$. This implies that V_M is proportional to $r_s^{-\frac{1}{4}M-1}$ as R_{mn} and $\omega_{\boldsymbol{k}\lambda}$ are proportional to r_s and $r_s^{-3/2}$, respectively, and V_M is independent of α. On the basis of perturbation theory we can then conclude that the ground state energy of (V.12) is a power series in $r_s^{-1/4}$ with the additional property that all odd powers of $r_s^{-1/4}$ do not appear.

Appendix VI

The ground state of the low density electron system can be expressed as (cf. (4.13))

$$|\psi_0\rangle = \sum_{\substack{\jmath_1,\ldots,\jmath_{2N} \\ \sigma_1,\ldots,\sigma_{2N}}} A^{\sigma_1\ldots\sigma_{2N}}_{\jmath_1\ldots\jmath_{2N}}(0)\, d^+_{\jmath_1\sigma_1}(\boldsymbol{R}_1),\ldots,d^+_{\jmath_{2N}\sigma_{2N}}(\boldsymbol{R}_{2N})|\rangle\ . \tag{VI.1}$$

Up to order $r_s^{-3/2}$ the coefficients $A^{\sigma_1\ldots\sigma_{2N}}_{\jmath_1\ldots\jmath_{2N}}(0)$ are determined by the requirement

$$A_{\boldsymbol{k}\lambda}|\psi_0\rangle = 0\ , \tag{VI.2}$$

for all $\boldsymbol{k}$ and λ. The operators $A_{\boldsymbol{k}\lambda}$ are given by, according to (4.31), (4.40), (4.47), (4.51) and (4.54),

$$A_{\boldsymbol{k}\lambda} = \frac{1}{\sqrt{2N}} \sum_{i,\hat{\boldsymbol{\xi}},\jmath,\sigma} \left[\alpha^{\boldsymbol{k}\lambda}_{i\hat{\boldsymbol{\xi}}}\, d^+_{\jmath+\hat{\boldsymbol{\xi}}\sigma}(\boldsymbol{R}_i)\, d_{\jmath\sigma}(\boldsymbol{R}_i) + \beta^{\boldsymbol{k}\lambda}_{i\hat{\boldsymbol{\xi}}}\, d^+_{\jmath\sigma}(\boldsymbol{R}_i)\, d_{\jmath+\hat{\boldsymbol{\xi}}\sigma}(\boldsymbol{R}_i)\right] \sqrt{(\jmath\cdot\hat{\boldsymbol{\xi}}+1)}\ , \tag{VI.3}$$

with

$$\begin{aligned} \alpha^{\boldsymbol{k}\lambda}_{i\hat{\boldsymbol{\xi}}} &= \left(\left[\frac{m\omega_{\boldsymbol{k}\lambda}\alpha}{2\hbar}\right]^{\frac{1}{2}} + \left[\frac{\hbar}{8m\omega_{\boldsymbol{k}\lambda}\alpha}\right]^{\frac{1}{2}}\right) e^{i\boldsymbol{k}\cdot\boldsymbol{R}_i}\,\boldsymbol{\epsilon}_{\boldsymbol{k}\lambda}\cdot\hat{\boldsymbol{\xi}}\ , \\ \beta^{\boldsymbol{k}\lambda}_{i\hat{\boldsymbol{\xi}}} &= \left(\left[\frac{m\omega_{\boldsymbol{k}\lambda}\alpha}{2\hbar}\right]^{\frac{1}{2}} - \left[\frac{\hbar}{8m\omega_{\boldsymbol{k}\lambda}\alpha}\right]^{\frac{1}{2}}\right) e^{i\boldsymbol{k}\cdot\boldsymbol{R}_i}\,\boldsymbol{\epsilon}_{\boldsymbol{k}\lambda}\cdot\hat{\boldsymbol{\xi}}\ . \end{aligned} \tag{VI.4}$$

Substituting (VI.3) into (VI.2) we obtain

$$\begin{aligned} \sum_{i,\hat{\boldsymbol{\xi}}} \sum_{\substack{\jmath_1,\ldots,\jmath_{2N} \\ \sigma_1,\ldots,\sigma_{2N}}} \Bigg[& A^{\sigma_1\ldots\sigma_{2N}}_{\jmath_1\ldots\jmath_i-\hat{\boldsymbol{\xi}}\ldots\jmath_{2N}}(0)\sqrt{(\jmath_i\cdot\hat{\boldsymbol{\xi}})}\ \alpha^{\boldsymbol{k}\lambda}_{i\hat{\boldsymbol{\xi}}} \\ & + A^{\sigma_1\ldots\sigma_{2N}}_{\jmath_1\ldots\jmath_i+\hat{\boldsymbol{\xi}}\ldots\jmath_{2N}}(0)\sqrt{(\jmath_i\cdot\hat{\boldsymbol{\xi}}+1)}\ \beta^{\boldsymbol{k}\lambda}_{i\hat{\boldsymbol{\xi}}}\Bigg] d^+_{\jmath_1\sigma_1}(\boldsymbol{R}_1),\ldots,d^+_{\jmath_{2N}\sigma_{2N}}(\boldsymbol{R}_{2N})|\rangle = 0\ , \end{aligned} \tag{VI.5}$$

for all $\boldsymbol{k}$ and λ. Thus for all sets $\{\jmath_1,\ldots,\jmath_{2N}\}$ and $\{\sigma_1,\ldots,\sigma_{2N}\}$ we have the following $6N$ linear equations:

$$\sum_{i,\hat{\xi}} \left[\sqrt{(\jmath_i \cdot \hat{\xi})}\, \alpha^{k\lambda}_{i\hat{\xi}}\, A^{\sigma_1 \ldots \sigma_{2N}}_{\jmath_1 \ldots \jmath_i - \hat{\xi} \ldots \jmath_{2N}}(0) + \sqrt{(\jmath_i \cdot \hat{\xi} + 1)}\, \beta^{k\lambda}_{i\hat{\xi}}\, A^{\sigma_1 \ldots \sigma_{2N}}_{\jmath_1 \ldots \jmath_i + \hat{\xi} \ldots \jmath_{2N}}(0) \right] = 0, \quad \text{(VI.6)}$$

for all k and λ.

These equations give rise to recursion relations between coefficients $A^{\sigma_1 \ldots \sigma_{2N}}_{\jmath_1 \ldots \jmath_{2N}}(0)$ with different $j = \sum_{i,\hat{\xi}} \jmath_i \cdot \hat{\xi}$ starting with $j = 0$ and $j = 1$. The complexity of these relations increases with increasing j and actually prevents a calculation of all coefficients. Nevertheless a few conclusions can be drawn from (VI.6).

(1) The coefficients with j odd are all zero. This can easily be seen for $j = 1$ by substituting $\jmath_1 = \jmath_2 = \ldots = \jmath_{2N} = 0$ into (VI.6). As the recursion relations only contain coefficients with $j = j_0$ and $j = j_0 + 2$, $j_0 = 1, 2, 3, \ldots$, all coefficients with j odd must be zero.

(2) The coefficients $A^{\sigma_1 \ldots \sigma_{2N}}_{\jmath_1 \ldots \jmath_{2N}}(0)$ with j even can all be expressed in terms of $A^{\sigma_1 \ldots \sigma_{2N}}_{0 \ldots 0}(0)$. They decrease as $[(\jmath_i \cdot \hat{\xi})!]^{-\frac{1}{2}}$ with increasing $\jmath_i \cdot \hat{\xi}$, $i = 1, \ldots, 2N$. The coefficients $A^{\sigma_1 \ldots \sigma_{2N}}_{0 \ldots 0}(0)$ can be chosen almost completely arbitrarily, the only restriction being that the ground state must be normalized. This means that the ground state is degenerate with respect to all possible spin configurations $\{\sigma_1, \ldots, \sigma_{2N}\}$ of the lattice. As discussed in section 3 this is due to the neglect of exchange contributions to the ground state energy.

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London stressed that a Meissner-Ochsenfeld effect can occur as soon as the system's wave function is rigid in the sense that it is hardly affected by a magnetic field.

II A description of the high-density electron system in terms of bosons *

Abstract

Tomonaga's idea of describing the one-dimensional jellium model in terms of bosons is adopted for the three-dimensional case, but worked out in a completely different way. An algorithm is given for the construction of a boson Hamiltonian that takes into account the full dynamics of the jellium model at all densities.
The algorithm is applied to a reduced form of the jellium model, that has the same ground state energy as the jellium model in the high-density limit. The resulting boson Hamiltonian is compared with Sawada's Hamiltonian, which also has this ground state energy in the limit of high-density. Finally, the present boson formulation is discussed briefly.

1. Introduction

The system of interacting electrons moving against a uniform background of neutralizing positive charge is known as the jellium model. Until now the ground state properties of the jellium model can only be calculated approximately except in the limiting cases of extremely high and low densities.

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Several ways of approach exist for dealing with the electron system. One of them is to reformulate this system in terms of bosons. The boson formulation of the one-dimensional model has been discussed by Tomonaga [1]. His formulation holds in the high-density limit, as then only scattering processes with small momentum transfer are important. The three-dimensional system has been discussed by Sawada in terms of a free boson Hamiltonian [2]. His purpose was the justification of the ground state energy calculation by Gell-Mann and Brueckner [3], who summed an apparently divergent series of ring diagrams. That calculation, which is equivalent to the Random Phase Approximation of Bohm and Pines [4], leads to the exact ground state energy in the high-density limit. Sawada's Hamiltonian is the result of discarding all interaction terms that do not generate ring diagrams. Consequently Sawada's boson description is only equivalent to the fermion description within the framework of perturbation theory. This means that Sawada's three-dimensional approach is not analogous to Tomanaga's formulation, as the latter one takes into account the full dynamics of the one-dimensional system in the high-density limit. The results of Arponen and Pajanne [5], who generalized Sawada's Hamiltonian and obtained a boson Hamiltonian, which is non-hermitian and of sixth order in the boson operators, support this conclusion.

The purpose of the present paper is to obtain a Tomonaga-like boson-formulation of the three-dimensional fermion system. In section 2 the algorithm is given for the construction of a boson Hamiltonian H_B, that takes into account the full dynamics of the jellium model at all densities. In section 3 this algorithm is applied to a reduced form of the jellium model, that has the same ground state energy as the jellium model in the high-density limit. The resulting boson Hamiltonian is compared with Sawada's Hamiltonian. Unlike Sawada's expression the present one describes a fermion system and can therefore be considered as a three-dimensional analogue of Tomonaga's Hamiltonian. The significance of the present boson formulation is discussed in section 4. Finally it should be remarked that the present paper can be considered as a logical continuation of a previous treatise on the boson formulation of the low-density electron system [6].

2. The Boson formulation

The plane wave representation of the jellium model is given by the Hamiltonian

$$H = \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}}\, c^{+}_{\boldsymbol{k}\sigma}\, c_{\boldsymbol{k}\sigma} + \frac{1}{2} \sum_{\substack{\boldsymbol{q},\boldsymbol{k},\boldsymbol{k}' \\ \sigma,\sigma'}}{}' V(\boldsymbol{q})\, c^{+}_{\boldsymbol{k}\sigma}\, c^{+}_{\boldsymbol{k}'\sigma'}\, c_{\boldsymbol{k}'+\boldsymbol{q}\sigma'}\, c_{\boldsymbol{k}-\boldsymbol{q}\sigma}\ , \tag{2.1}$$

where

$$V(\boldsymbol{q}) = \frac{4\pi e^2}{\Omega q^2}\ , \tag{2.2}$$

and

$$\epsilon_{\boldsymbol{k}} = \frac{\hbar^2 k^2}{2m}\ . \tag{2.3}$$

Here e and m are the charge and mass of an electron, respectively, and Ω denotes the volume of the system, that is thought to consist of $2N$ electrons. The operators $c_{\boldsymbol{k}\sigma}$ and $c^{+}_{\boldsymbol{k}\sigma}$ describe the annihilation and creation of a fermion having wave vector $\boldsymbol{k}$ and spin σ, respectively. The prime appearing in the summation over the momentum transfers $\boldsymbol{q}$ indicates that the $\boldsymbol{q} = 0$ term is excluded in consequence of the homogeneous positively charged background.

The first step of the present boson formulation for the jellium model concerns the calculation of the matrix elements of the jellium model using the complete set of eigenstates of the kinetic energy operator appearing in (2.1). An eigenstate $|m\rangle$ of this set can be expressed as

$$|m\rangle = \left(\prod_{i=1}^{m} \theta(k_F - |\boldsymbol{k}_i|)\ \theta(|\boldsymbol{k}_i + \boldsymbol{q}_i| - k_F)\ c^{+}_{\boldsymbol{k}_i+\boldsymbol{q}_i\tau_i} c_{\boldsymbol{k}_i\sigma_i} \right) |0\rangle\ , \tag{2.4}$$

where $|0\rangle$, the filled Fermi sphere, is the ground state of the kinetic energy operator and k_F denotes the radius of the Fermi sphere. The matrix elements can be easily calculated. The diagonal element $\langle m|H|m\rangle$ is given by

$$\langle m|H|m\rangle = \sum_{\boldsymbol{k}\sigma} \left[\epsilon_{\boldsymbol{k}} - \frac{1}{2} \sum_{\boldsymbol{q}}{}' \; V(\boldsymbol{q}) \langle m|n_{\boldsymbol{k}+\boldsymbol{q}\sigma}|m\rangle \right] \langle m|n_{\boldsymbol{k}\sigma}|m\rangle \; , \tag{2.5}$$

where

$$\langle m|n_{\boldsymbol{k}\sigma}|m\rangle = \langle m|c^{+}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma}|m\rangle = \begin{cases} 1 & \text{if } |\boldsymbol{k}| < k_F \text{ and } (\boldsymbol{k},\sigma) \neq (\boldsymbol{k}_i,\sigma_i); \\ 1 & \text{if } |\boldsymbol{k}| > k_F \text{ and } (\boldsymbol{k},\sigma) = (\boldsymbol{k}_i+\boldsymbol{q}_i,\tau_i); \\ 0 & \text{otherwise .} \end{cases} \tag{2.6}$$

The off-diagonal element $\langle m|H|m'\rangle$ is zero unless $|m'\rangle$ is of the following form:

$$|m'\rangle = c^{+}_{\boldsymbol{\ell}_4\tau'_2} c_{\boldsymbol{\ell}_2\tau_2} c^{+}_{\boldsymbol{\ell}_3\tau'_1} c_{\boldsymbol{\ell}_1\tau_1}|m\rangle \; , \tag{2.7}$$

where the creation and annihilation operators refer to four mutually different one-electron states. This is a direct consequence of the two-body nature of the interaction term in (2.1). The non-zero matrix element $\langle m|H|m'\rangle$ is given by

$$\langle m|H|m'\rangle = [V(\boldsymbol{\ell}_1 - \boldsymbol{\ell}_3)\delta_{\tau_1\tau'_1}\delta_{\tau_2\tau'_2} - V(\boldsymbol{\ell}_2 - \boldsymbol{\ell}_3)\delta_{\tau_2\tau'_1}\delta_{\tau_1\tau'_2}]\delta_{\boldsymbol{\ell}_1+\boldsymbol{\ell}_2,\boldsymbol{\ell}_3+\boldsymbol{\ell}_4} \; . \tag{2.8}$$

Next the matrix elements (2.8) are used as the guiding principle for the formulation of the jellium model in terms of a boson Hamiltonian H_B. In order to construct H_B each fermion state $|m\rangle$ is replaced by a corresponding boson state $|\varphi_{Am}\rangle$. The set of boson states that corresponds with the complete set of fermion states is obtained by replacing each electron-hole pair $c^{+}_{\boldsymbol{k}+\boldsymbol{q}\sigma'} c_{\boldsymbol{k}\sigma}$ with $|\boldsymbol{k}+\boldsymbol{q}| > k_F$ and $|\boldsymbol{k}| < k_F$ by the corresponding boson operator $d^{+}_{\boldsymbol{q}\sigma'}(\boldsymbol{k}\sigma)$. The boson operators satisfy the commutation relations

$$[d^{+}_{\boldsymbol{q}\sigma'}(\boldsymbol{k}\sigma), d^{+}_{\boldsymbol{q}'\tau'}(\boldsymbol{k}'\tau)] = 0 \; ,$$

$$[d_{\boldsymbol{q}\sigma'}(\boldsymbol{k}\sigma), d^{+}_{\boldsymbol{q}'\tau'}(\boldsymbol{k}'\tau)] = \delta_{\boldsymbol{q}\boldsymbol{q}'}\,\delta_{\boldsymbol{k}\boldsymbol{k}'}\,\delta_{\sigma\tau}\,\delta_{\sigma'\tau'}\ . \tag{2.9}$$

The replacement means that the fermion state $|m\rangle$ (2.4) corresponds with the boson state

$$|\varphi_{Am}\rangle = \left(\prod_{i=1}^{m}\ \theta(k_F - |\boldsymbol{k}_i|)\ \ \theta(|\boldsymbol{k}_i + \boldsymbol{q}_i| - k_F)\ \ d^{+}_{\boldsymbol{q}_i\tau_i}(\boldsymbol{k}_i\sigma_i)\right)|\varphi_{A0}\rangle\ , \tag{2.10}$$

where $|\varphi_{A0}\rangle$ is the vacuum state for the bosons, i.e.

$$d_{\boldsymbol{q}\sigma'}(\boldsymbol{k}\sigma)|\varphi_{A0}\rangle = 0 \tag{2.11}$$

for all $\boldsymbol{q}, \boldsymbol{k}, \sigma'$ and σ. Note that the restrictions $|\boldsymbol{k}_i| < k_F$ and $|\boldsymbol{k}_i + \boldsymbol{q}_i| > k_F$ in (2.10) are superfluous, as the operators $d^{+}_{\boldsymbol{q}\sigma'}(\boldsymbol{k}\sigma)$ are defined for $|\boldsymbol{k}| < k_F$ and $|\boldsymbol{k} + \boldsymbol{q}| > k_F$ only. Consequently they will no longer be mentioned explicitly.

Clearly the number of boson states that can be constructed in terms of the boson creation operator $d^{+}_{\boldsymbol{q}\sigma'}(\boldsymbol{k}\sigma)$ and the vacuum state $|\varphi_{A0}\rangle$ exceeds by far the number of fermion states. For instance a boson state like

$$|\varphi_{C2}\rangle = d^{+}_{\boldsymbol{q}_1\tau_1}(\boldsymbol{k}_1\sigma_1)d^{+}_{\boldsymbol{q}_2\tau_2}(\boldsymbol{k}_1\sigma_1)|\varphi_{A0}\rangle \tag{2.12}$$

does not correspond with any fermion state, whereas a boson state like

$$|\varphi_{B2}\rangle = -d^{+}_{\boldsymbol{q}_1+\boldsymbol{k}_1-\boldsymbol{k}_2\tau_1}(\boldsymbol{k}_2\sigma_2)d^{+}_{\boldsymbol{q}_2+\boldsymbol{k}_2-\boldsymbol{k}_1\tau_2}(\boldsymbol{k}_1\sigma_1)|\varphi_{A0}\rangle \tag{2.13}$$

corresponds with the same fermion state as the boson state $|\varphi_{A2}\rangle$ defined in (2.10). For clearness' sake the complete set of boson states is divided up into three subsets A, B and C. Subset A consists of states $|\varphi_{Am}\rangle$ being in a one-to-one correspondence with the complete set of fermion states $|m\rangle$ (2.4). Subset B consists of those boson states $|\varphi_{Bm}\rangle$ that correspond with fermion states already taken into account by the states $|\varphi_{Am}\rangle$ (cf. 2.13). Finally subset C consists of boson states which do not correspond with any fermion state (cf. 2.12).

Now the boson Hamiltonian H_B is constructed by requiring

$$\begin{aligned} \langle\varphi_{Am}|H_B|\varphi_{Am}\rangle &= \langle m|H|m\rangle, \\ \langle\varphi_{Am}|H_B|\varphi_{Am'}\rangle &= \langle m|H|m'\rangle, \end{aligned} \tag{2.14}$$

for all fermion states $|m\rangle$ and $|m'\rangle$, and further

$$\langle\varphi_{Am}|H_B|\varphi_{Bm'}\rangle = \langle\varphi_{Am}|H_B|\varphi_{Cm'}\rangle = 0 \tag{2.15}$$

for all boson states of the respective subsets. The correctness of this procedure follows immediately from the form of the matrix representation of H_B, $M(H_B)$, on the complete set of boson states:

$$M(H_B) = \begin{pmatrix} M_A & 0 \\ 0 & M_{BC} \end{pmatrix}, \tag{2.16}$$

where M_A is the matrix representation of H_B on the subset A, i.e. M_A is identical to the matrix representation of the jellium model, and M_{BC} is the matrix representation of H_B on the subset of the remaining boson states. Consequentely the boson system as described by H_B is not equivalent with the jellium model but includes that model. The merit of the present formulation is the separation of fermion and non-fermion states. This means that the eigenvalues of the jellium model form a subset of all eigenvalues of H_B. In this sense H_B can be said to describe the jellium model.

For constructional purposes H_B is written as

$$H_B = H_B^1 + H_B^2 + \Delta H_B, \tag{2.17}$$

where H_B^1, H_B^2 and ΔH_B are chosen such that

$$
\begin{aligned}
\langle\varphi_{Am}|H_B|\varphi_{Am}\rangle &= \langle\varphi_{Am}|H_B^1|\varphi_{Am}\rangle, \\
\langle\varphi_{Am}|H_B|\varphi_{Am'}\rangle &= \langle\varphi_{Am}|H_B^2|\varphi_{Am'}\rangle, \qquad m \neq m', \\
\langle\varphi_{Am}|H_B^1 + H_B^2|\varphi_{\mu m'}\rangle &= -\langle\varphi_{Am}|\Delta H_B|\varphi_{\mu m'}\rangle, \quad \mu = B, C.
\end{aligned}
\tag{2.18}
$$

First H_B^1 is constructed. Thereto the following boson operator is introduced:

$$
n_{\boldsymbol{k}\sigma}^B = \theta(k_F - k) + {\sum_{\boldsymbol{q}\sigma'}}' \left[d_{\boldsymbol{q}\sigma}^+(\boldsymbol{k} - \boldsymbol{q}\sigma')\, d_{\boldsymbol{q}\sigma}(\boldsymbol{k} - \boldsymbol{q}\sigma') - d_{\boldsymbol{q}\sigma'}^+(\boldsymbol{k}\sigma) d_{\boldsymbol{q}\sigma'}(\boldsymbol{k}\sigma)\right] \tag{2.19}
$$

It can be shown that:

(1) the boson states are eigenstates of $n_{\boldsymbol{k}\sigma}^B$ and

(2) $n_{\boldsymbol{k}\sigma}^B|\varphi_{Am}\rangle = n_{\boldsymbol{k}\sigma}|m\rangle$.

Consequently it holds:

$$
H_B^1 = \sum_{\boldsymbol{k}\sigma} [\epsilon_{\boldsymbol{k}} n_{\boldsymbol{k}\sigma}^B - \frac{1}{2} {\sum_{\boldsymbol{q}}}' V(\boldsymbol{q})\, n_{\boldsymbol{k}+\boldsymbol{q}\sigma}^B\, n_{\boldsymbol{k}\sigma}^B] \,. \tag{2.20}
$$

The term H_B^2 is obtained by expressing H_B^2 as

$$
H_B^2 = \sum_{i=1}^{9} H_B^2(i) \,, \tag{2.21}
$$

where the appearing nine terms $H_B^2(i)$ refer to the nine different types of off-diagonal matrix elements (2.8). These types are characterized by the signs of $|\boldsymbol{\ell}_j| - k_F$, $j = 1, 2, 3, 4$, where it must be taken into account that a permutation of $\boldsymbol{\ell}_1$ and $\boldsymbol{\ell}_2$ or $\boldsymbol{\ell}_3$ and $\boldsymbol{\ell}_4$ does not lead to a new type of matrix element. The nine types are:

(1) $|\boldsymbol{\ell}_1|,\ |\boldsymbol{\ell}_2|,\ |\boldsymbol{\ell}_3|,\ |\boldsymbol{\ell}_4| > k_F$;

(2) $|\boldsymbol{\ell}_1|,\ |\boldsymbol{\ell}_2|,\ |\boldsymbol{\ell}_3|,\ |\boldsymbol{\ell}_4| < k_F$;

$$(3)\quad |\boldsymbol{\ell}_1| < k_F \quad , \quad |\boldsymbol{\ell}_2|,\ |\boldsymbol{\ell}_3|,\ |\boldsymbol{\ell}_4| > k_F;$$

$$(4)\quad |\boldsymbol{\ell}_3| < k_F \quad , \quad |\boldsymbol{\ell}_1|,\ |\boldsymbol{\ell}_2|,\ |\boldsymbol{\ell}_4| > k_F;$$

$$(5)\quad |\boldsymbol{\ell}_1| > k_F \quad , \quad |\boldsymbol{\ell}_2|,\ |\boldsymbol{\ell}_3|,\ |\boldsymbol{\ell}_4| < k_F;$$

$$(6)\quad |\boldsymbol{\ell}_3| > k_F \quad , \quad |\boldsymbol{\ell}_1|,\ |\boldsymbol{\ell}_2|,\ |\boldsymbol{\ell}_4| < k_F;$$

$$(7)\quad |\boldsymbol{\ell}_1|,\ |\boldsymbol{\ell}_2| < k_F \quad , \quad |\boldsymbol{\ell}_3|,\ |\boldsymbol{\ell}_4| > k_F;$$

$$(8)\quad |\boldsymbol{\ell}_1|,\ |\boldsymbol{\ell}_2| < k_F \quad , \quad |\boldsymbol{\ell}_3|,\ |\boldsymbol{\ell}_4| < k_F;$$

$$(9)\quad |\boldsymbol{\ell}_1|,\ |\boldsymbol{\ell}_4| < k_F \quad , \quad |\boldsymbol{\ell}_2|,\ |\boldsymbol{\ell}_3| > k_F\ .$$

The construction of the terms $H_B^2(i), i = 1, \ldots, 9$ is straightforward. As an example the term $H_B^2(1)$ is constructed here. The translation of fermion states into corresponding boson states is facilitated by putting $\boldsymbol{\ell}_1 = \boldsymbol{k}_1 + \boldsymbol{q}_1$, $\boldsymbol{\ell}_2 = \boldsymbol{k}_2 + \boldsymbol{q}_2$, $\boldsymbol{\ell}_3 = \boldsymbol{k}_1 + \boldsymbol{q}_1'$, $\boldsymbol{\ell}_4 = \boldsymbol{k}_1 + \boldsymbol{q}_2'$ with $|\boldsymbol{k}_1|$, $|\boldsymbol{k}_2| < k_F$. Then the states $|m\rangle$ and $|m'\rangle$ as given by (2.4) and (2.7) can be expressed as follows:

$$\begin{aligned} |m\rangle &= c^+_{\boldsymbol{k}_1+\boldsymbol{q}_1\tau_1}\, c_{\boldsymbol{k}_1\sigma_1}\, c^+_{\boldsymbol{k}_2+\boldsymbol{q}_2\tau_2}\, c_{\boldsymbol{k}_2\sigma_2} |m-2\rangle\ , \\ |m'\rangle &= c^+_{\boldsymbol{k}_1+\boldsymbol{q}_1'\tau_1'}\, c_{\boldsymbol{k}_1\sigma_1}\, c^+_{\boldsymbol{k}_2+\boldsymbol{q}_2'\tau_2'}\, c_{\boldsymbol{k}_2\sigma_2} |m-2\rangle\ , \end{aligned} \tag{2.22}$$

where the appearing fermion operators refer to six mutually different fermion states and $|m-2\rangle$ is given by

$$|m-2\rangle = \left(\prod_{\iota=3}^{m} \theta(k_F - |\boldsymbol{k}_\iota|)\ \theta(|\boldsymbol{k}_\iota + \boldsymbol{q}_\iota| - k_F)\ c^+_{\boldsymbol{k}_\iota+\boldsymbol{q}_\iota\tau_\iota}\, c_{\boldsymbol{k}_\iota\sigma_\iota} \right) |0\rangle\ . \tag{2.23}$$

Clearly the corresponding boson states $|\varphi_{Am}\rangle$ and $|\varphi_{Am'}\rangle$ read:

$$
\begin{aligned}
|\varphi_{Am}\rangle &= d^{+}_{\boldsymbol{q}_1\tau_1}(\boldsymbol{k}_1\sigma_1)d^{+}_{\boldsymbol{q}_2\tau_2}(\boldsymbol{k}_2\sigma_2)|\varphi_{Am-2}\rangle \ , \\
|\varphi_{Am'}\rangle &= d^{+}_{\boldsymbol{q}'_1\tau'_1}(\boldsymbol{k}_1\sigma_1)d^{+}_{\boldsymbol{q}'_2\tau'_2}(\boldsymbol{k}_2\sigma_2)|\varphi_{Am-2}\rangle \ ,
\end{aligned}
\tag{2.24}
$$

where

$$
\begin{aligned}
d_{\boldsymbol{q}_1\tau_1}(\boldsymbol{k}_1\sigma_1)|\varphi_{Am-2}\rangle &= d_{\boldsymbol{q}_2\tau_2}(\boldsymbol{k}_2\sigma_2)|\varphi_{Am-2}\rangle = d_{\boldsymbol{q}'_1\tau'_1}(\boldsymbol{k}_1\sigma_1)|\varphi_{Am-2}\rangle \\
&= d_{\boldsymbol{q}'_2\tau'_2}(\boldsymbol{k}_2\sigma_2)|\varphi_{Am-2}\rangle = 0 \ .
\end{aligned}
\tag{2.25}
$$

The requirement (2.25) follows directly from the correspondence of $|\varphi_{Am-2}\rangle$ with the fermion state $|m-2\rangle$ given by (2.23). Using

$$
\begin{aligned}
\langle\varphi_{Am}|H^2_B(1)|\varphi_{Am'}\rangle &= [V(\boldsymbol{q}_1-\boldsymbol{q}'_1)\delta_{\tau_1\tau'_1}\delta_{\tau_2\tau'_2} \\
&- V(\boldsymbol{k}_2+\boldsymbol{q}_2-\boldsymbol{k}_1-\boldsymbol{q}'_1)\delta_{\tau_2\tau'_1}\delta_{\tau_1\tau'_2}]\delta_{\boldsymbol{q}_1+\boldsymbol{q}_2,\boldsymbol{q}'_1+\boldsymbol{q}'_2}
\end{aligned}
\tag{2.26}
$$

for any pair of boson states of the type given by (2.24), $H^2_B(1)$ is found to have the form

$$
\begin{aligned}
H^2_B(1) &= \frac{1}{2}\sum_{\boldsymbol{p}_1,\boldsymbol{p}_2,\boldsymbol{p}'_1,\boldsymbol{p}'_2,\tau,\tau'}{}' \quad \sum_{\boldsymbol{k},\boldsymbol{k}',\sigma,\sigma'}{}' \quad \delta_{\boldsymbol{p}_1+\boldsymbol{p}_2,\boldsymbol{p}'_1+\boldsymbol{p}'_2}\Big[\\
&V(\boldsymbol{p}_1-\boldsymbol{p}'_1)\, d^{+}_{\boldsymbol{p}_1\tau}(\boldsymbol{k}\sigma)\, d^{+}_{\boldsymbol{p}_2\tau'}(\boldsymbol{k}'\sigma')\, d_{\boldsymbol{p}'_1\tau}(\boldsymbol{k}\sigma)\, d_{\boldsymbol{p}'_2\tau'}(\boldsymbol{k}'\sigma') \\
&- V(\boldsymbol{k}'+\boldsymbol{p}_2-\boldsymbol{k}-\boldsymbol{p}'_1)\, d^{+}_{\boldsymbol{p}_1\tau}(\boldsymbol{k}\sigma)\, d^{+}_{\boldsymbol{p}_2\tau'}(\boldsymbol{k}'\sigma')\, d_{\boldsymbol{p}'_1\tau'}(\boldsymbol{k}\sigma)\, d_{\boldsymbol{p}'_2\tau}(\boldsymbol{k}'\sigma') \Big] \ ,
\end{aligned}
\tag{2.27}
$$

where the primes appearing in the summations indicate that terms containing $V(0)$ are excluded as well as that the boson operators must be such that the corresponding fermion operators are all different. Note further that the relevant matrix elements of $H^2_B(1)$

between the boson states of subset A are indeed all zero except for those pairs of states as given by (2.24). Consequently $H_B^2(1)$ is correctly expressed by (2.27).

The remaining terms of $H_B^2(1)$ (2.21) can be constructed analogous to $H_B^2(1)$. They are found to be

$$H_B^2(2) = \frac{1}{2} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_1',\boldsymbol{k}_2'\tau,\tau'}{}' \quad \sum_{\boldsymbol{q},\boldsymbol{q}'\sigma,\sigma'}{}' \quad \delta_{\boldsymbol{k}_1+\boldsymbol{k}_2,\boldsymbol{k}_1'+\boldsymbol{k}_2'} \Big[\tag{2.28}$$

$$V(\boldsymbol{k}_1-\boldsymbol{k}_1')\, d^+_{\boldsymbol{q}+\boldsymbol{k}_1'-\boldsymbol{k}_1\sigma}(\boldsymbol{k}_1\tau)\, d^+_{\boldsymbol{q}'+\boldsymbol{k}_2'-\boldsymbol{k}_2\sigma'}(\boldsymbol{k}_2\tau')\, d_{\boldsymbol{q}\sigma}(\boldsymbol{k}_1'\tau)\, d_{\boldsymbol{q}'\sigma'}(\boldsymbol{k}_2'\tau')$$

$$- V(\boldsymbol{k}_2-\boldsymbol{k}_1')\, d^+_{\boldsymbol{q}+\boldsymbol{k}_1'-\boldsymbol{k}_1\sigma}(\boldsymbol{k}_1\tau)\; d^+_{\boldsymbol{q}'+\boldsymbol{k}_2'-\boldsymbol{k}_2\sigma'}(\boldsymbol{k}_2\tau')\, d_{\boldsymbol{q}\sigma}(\boldsymbol{k}_1'\tau')\, d_{\boldsymbol{q}'\sigma'}(\boldsymbol{k}_2'\tau)\Big] \ ,$$

$$H_B^2(3) = \sum_{\boldsymbol{q},\boldsymbol{p},\boldsymbol{p}',\tau}{}' \quad \sum_{\boldsymbol{k},\boldsymbol{k}',\sigma,\sigma'}{}' \Big[V(\boldsymbol{q})\, d^+_{\boldsymbol{p}'\tau}(\boldsymbol{k}'\sigma')\, d^+_{\boldsymbol{q}\sigma}(\boldsymbol{k}\sigma)\, d_{\boldsymbol{p}\tau}(\boldsymbol{k}'\sigma')$$

$$- V(\boldsymbol{p}'+\boldsymbol{k}'-\boldsymbol{k})\, d^+_{\boldsymbol{p}'\sigma}(\boldsymbol{k}'\sigma')\, d^+_{\boldsymbol{q}\tau}(\boldsymbol{k}\sigma)\, d_{\boldsymbol{p}\tau}(\boldsymbol{k}'\sigma')\Big]\, \delta_{\boldsymbol{p},\boldsymbol{q}+\boldsymbol{p}'} \ , \tag{2.29}$$

$$H_B^2(4) = \Big[H_B^2(3)\Big]^+ \ , \tag{2.30}$$

$$H_B^2(5) = \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_1',\tau}{}' \quad \sum_{\boldsymbol{q},\boldsymbol{q}',\sigma,\sigma'}{}' \Big[V(\boldsymbol{q}')\, d^+_{\boldsymbol{q}+\boldsymbol{k}_1'-\boldsymbol{k}_2\sigma}(\boldsymbol{k}_2\tau)\, d_{\boldsymbol{q}\sigma}(\boldsymbol{k}_1'\tau)\, d_{\boldsymbol{q}'\sigma'}(\boldsymbol{k}_1\sigma')$$

$$- V(\boldsymbol{k}_2-\boldsymbol{k}_1)\, d^+_{\boldsymbol{q}+\boldsymbol{k}_1'-\boldsymbol{k}_2\sigma}(\boldsymbol{k}_2\tau)\, d_{\boldsymbol{q}\sigma}(\boldsymbol{k}_1'\sigma')\, d_{\boldsymbol{q}'\sigma'}(\boldsymbol{k}_1\tau)\Big]\, \delta_{\boldsymbol{q}'+\boldsymbol{k}_2,\boldsymbol{k}_1'} \ , \tag{2.31}$$

$$H_B^2(6) = [H_B^2(5)]^+ \ , \tag{2.32}$$

$$H_B^2(7) = \frac{1}{2} \sum_{\boldsymbol{q},\boldsymbol{k},\boldsymbol{k}',\sigma,\sigma'}{}' \quad \Big[V(\boldsymbol{q})\, d^+_{-\boldsymbol{q}\sigma'}(-\boldsymbol{k}'\sigma')\, d^+_{\boldsymbol{q}\sigma}(\boldsymbol{k}\sigma)$$

$$-V(\boldsymbol{q}+\boldsymbol{k}+\boldsymbol{k}')\, d^+_{-\boldsymbol{q}\sigma'}(-\boldsymbol{k}'\sigma)\, d^+_{\boldsymbol{q}\sigma}(\boldsymbol{k}\sigma')\Big] \ , \tag{2.33}$$

$$H_B^2(8) \;=\; \left[H_B^2(7)\right]^+ \;, \tag{2.34}$$

$$H_B^2(9) \;=\; {\sum_{\boldsymbol{q},\boldsymbol{k},\boldsymbol{k}'\sigma,\sigma'}}' \left[V(\boldsymbol{q})\, d^+_{\boldsymbol{q}\sigma'}(\boldsymbol{k}'\sigma')\, d_{\boldsymbol{q}\sigma}(\boldsymbol{k}\sigma) - V(\boldsymbol{k}-\boldsymbol{k}')\, d^+_{\boldsymbol{q}\sigma}(\boldsymbol{k}'\sigma')\, d_{\boldsymbol{q}\sigma}(\boldsymbol{k}\sigma')\right] \;. \tag{2.35}$$

The primes appearing in the summations indicate that the terms with $V(0)$ are excluded as well as that the appearing boson operators must be such that the corresponding fermion operators are all different.

The construction of the remaining term ΔH_B of the boson Hamiltonian H_B (2.17) is in principle straightforward as well. For instance matrix elements like $\langle\varphi_{Am}|H_B^1 + H_B^2|\varphi_{Cm+2}\rangle$, with

$$\begin{aligned} |\varphi_{Am}\rangle &= d^+_{\boldsymbol{q}_3\sigma_3}(\boldsymbol{k}_1\sigma_1')|\varphi_{Am-1}\rangle \;, \\ |\varphi_{Cm+2}\rangle &= d^+_{\boldsymbol{q}_2\sigma_2}(\boldsymbol{k}_2\sigma_2')\, d^+_{\boldsymbol{q}_1\sigma_1}(\boldsymbol{k}_1\sigma_1')\, d^+_{\boldsymbol{q}_3\sigma_3}(\boldsymbol{k}_1\sigma_1')|\varphi_{Am-1}\rangle \;, \end{aligned} \tag{2.36}$$

are compensated by matrix elements $\langle\varphi_{Am}|\Delta h_B|\varphi_{Cm+2}\rangle$, where

$$\Delta h_B = -{\sum_{\boldsymbol{q},\boldsymbol{q}'\boldsymbol{k},\boldsymbol{k}'\sigma,\sigma'\tau}}' d^+_{\boldsymbol{q}'\tau}(\boldsymbol{k}\sigma) d_{\boldsymbol{q}'\tau}(\boldsymbol{k}\sigma) \left[V(\boldsymbol{q}) d_{\boldsymbol{q}\sigma}(\boldsymbol{k}\sigma) d_{-\boldsymbol{q}\sigma'}(-\boldsymbol{k}'\sigma') - V(\boldsymbol{q}+\boldsymbol{k}+\boldsymbol{k}') d_{\boldsymbol{q}\sigma'}(\boldsymbol{k}\sigma) d_{-\boldsymbol{q}\sigma}(-\boldsymbol{k}'\sigma')\right] \tag{2.37}$$

is one of the terms of ΔH_B. The remaining terms of ΔH_B, which must compensate matrix elements of the type $\langle\varphi_{Am}|H_B^1 + H_B^2|\varphi_{Cm'}\rangle$ can be found analogously. The compensation of matrix elements of the type $\langle\varphi_{Am}|H_B^1 + H_B^2|\varphi_{Bm'}\rangle$ can in principle be brought about

by imposing additional restrictions on the summations in (2.27) - (2.35). E.g. a matrix-element like $\langle\varphi_{A0}|H_B^1 + H_B^2 + \Delta H_B|\varphi_{B2}\rangle$, where $|\varphi_{B2}\rangle$ is given by (2.13), is zero if the summation in (2.34) is further restricted by requiring that the term proportional to $-d_{-\boldsymbol{q}_1+\boldsymbol{k}_2-\boldsymbol{k}_1\tau_2}(\boldsymbol{k}_1\sigma_1)d_{\boldsymbol{q}_1+\boldsymbol{k}_1-\boldsymbol{k}_2\tau_1}(\boldsymbol{k}_2\sigma_2)$ is not taken into account.

3. The high-density limit

The boson Hamiltonian H_B, which includes the full description of the jellium model at all densities, cannot be constructed explicitly due to the complexity of ΔH_B. The algorithm given in section 2, however, can be applied to simpler fermion systems, which allow an explicit description in terms of bosons. Here the algorithm of section 2 is applied to a reduced form H_F of the jellium model, which has the same ground state energy as the jellium model in the high-density limit.

Starting point of the present analysis is the following fermion Hamiltonian:

$$\begin{aligned}\tilde{H}_F &= \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}} c^+_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} - \frac{1}{2} {\sum_{\boldsymbol{k},\boldsymbol{q},\sigma}}' V(\boldsymbol{q})\theta(k_F-k)\theta(k_F-|\boldsymbol{k}+\boldsymbol{q}|) \\ &+ \frac{1}{2} {\sum_{\boldsymbol{q},\boldsymbol{k},\boldsymbol{k}',\sigma,\sigma'}}' \theta(k_F-k)\theta(k_F-k')\theta(|\boldsymbol{k}+\boldsymbol{q}|-k_F)\theta(|\boldsymbol{k}'+\boldsymbol{q}|-k_F)V(\boldsymbol{q}) \Big[\\ &\Big[c^+_{-\boldsymbol{k}'-\boldsymbol{q}\sigma'} c_{-\boldsymbol{k}'\sigma'} + c^+_{\boldsymbol{k}'\sigma'} c_{\boldsymbol{k}'+\boldsymbol{q}\sigma'}\Big] \Big[c^+_{\boldsymbol{k}+\boldsymbol{q}\sigma} c_{\boldsymbol{k}\sigma} + c^+_{-\boldsymbol{k}\sigma} c_{-\boldsymbol{k}-\boldsymbol{q}\sigma}\Big]\Big] \,. \end{aligned} \tag{3.1}$$

As shown by Sawada [2] $\tilde{H}_F$ has the ground state energy of the jellium model in the high-density limit [3], namely

$$E_0 = 2N\left[\frac{2.2}{r_s^2} - \frac{0.9}{r_s} + 0.0622 \ln r_s\right] , \tag{3.2}$$

where E_0 is given in Rydberg and the dimensionless parameter r_s is given by

$$r_s = \left(\frac{3\Omega}{8\pi N}\right)^{1/3} \frac{me^2}{\hbar^2}. \tag{3.3}$$

Sawada's Hamiltonian H_S is obtained by simply replacing the fermion pair operator $c^+_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}\sigma}$ by the boson operator $n^B_{\boldsymbol{k}\sigma}$ (2.19) and the electron-hole pair $c^+_{\boldsymbol{k}+\boldsymbol{q}\sigma}c_{\boldsymbol{k}\sigma}$ with $|\boldsymbol{k}+\boldsymbol{q}| > k_F$ and $k < k_F$ by the boson operator $d^+_{\boldsymbol{q}\sigma}(\boldsymbol{k}\sigma)$, i.e.

$$\begin{aligned} H_S &= \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}} n^B_{\boldsymbol{k}\sigma} - \frac{1}{2} {\sum_{\boldsymbol{k},\boldsymbol{q},\sigma}}' V(\boldsymbol{q})\theta(k_F - k)\theta(k_F - |\boldsymbol{k}+\boldsymbol{q}|) \\ &+ \frac{1}{2} {\sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q},\sigma,\sigma'}}' V(\boldsymbol{q}) \left[d^+_{-\boldsymbol{q}\sigma'}(-\boldsymbol{k}'\sigma') + d_{\boldsymbol{q}\sigma'}(\boldsymbol{k}'\sigma')\right]\Big[\\ &\qquad d^+_{\boldsymbol{q}\sigma}(\boldsymbol{k}\sigma) + d_{-\boldsymbol{q}\sigma}(-\boldsymbol{k}\sigma)\Big] \,, \end{aligned} \tag{3.4}$$

Clearly H_S does not describe a fermion system, as the eigenstates of H_S are linear combinations of states belonging to the subsets A, B and C.

The fermion Hamiltonian $\tilde{H}_F$ (3.1) still contains too many terms for the present purpose of describing the fermion system (3.1) in terms of bosons. Notably interaction terms with large momentum transfer $q \gtrsim k_F$, that do not contribute to the ground state energy in the high-density limit (3.2) as shown in the appendix, prevent an explicit description of the fermion system in terms of bosons. For that reason the algorithm of section 2 is not applied to $\tilde{H}_F$ itself but to a reduced form of $\tilde{H}_F$ leaving out interaction terms with $q \gtrsim k_F$. This reduced form is the following fermion Hamiltonian:

$$\begin{aligned} H_F &= \sum_{\boldsymbol{k},\sigma} \epsilon_{\boldsymbol{k}} c^+_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} - \frac{1}{2} {\sum_{\boldsymbol{k},\boldsymbol{q},\sigma}}' V(\boldsymbol{q})\theta(k_F - k)\theta(k_F - |\boldsymbol{k}+\boldsymbol{q}|) \\ &+ \frac{1}{2} {\sum_{\boldsymbol{q},\boldsymbol{k},\boldsymbol{k}',\sigma,\sigma'}}'' \theta(k_F - k)\theta(k_F - k')\theta(|\boldsymbol{k}+\boldsymbol{q}| - k_F)\theta(|\boldsymbol{k}'+\boldsymbol{q}| - k_F) V(\boldsymbol{q}) \Big[\end{aligned}$$

$$\left[c^+_{-\boldsymbol{k}'-\boldsymbol{q}\sigma'}c_{-\boldsymbol{k}'\sigma'} + c^+_{\boldsymbol{k}'\sigma'}c_{\boldsymbol{k}'+\boldsymbol{q}\sigma'}\right]\left[c^+_{\boldsymbol{k}+\boldsymbol{q}\sigma}c_{\boldsymbol{k}\sigma} + c^+_{-\boldsymbol{k}\sigma}c_{-\boldsymbol{k}-\boldsymbol{q}\sigma}\right]\Big] \,, \tag{3.5}$$

where the double prime appearing in the second summation over $\boldsymbol{q}$ indicates that this summation is restricted to those terms satisfying $0 < q < r_s^{1/4}k_F < |\boldsymbol{q}+\boldsymbol{k}+\boldsymbol{k}'|$.
The restriction $q < r_s^{1/4}k_F < |\boldsymbol{q}+\boldsymbol{k}'+\boldsymbol{k}|$ must be imposed in order to obtain an explicit description of H_F in terms of bosons, as shown in the following. The influence of this restriction on the ground state energy in the high-density limit ($r_s \to 0$) is negligible (see Appendix).

The boson Hamiltonian H_{FB}, which describes the fermion system defined by (3.5), is now obtained from the fermion Hamiltonian H_F by requiring

$$\begin{aligned} \langle\varphi_{Am}|H_{FB}|\varphi_{Am'}\rangle &= \langle m|H_F|m'\rangle, \\ \langle\varphi_{Am}|H_{FB}|\varphi_{Bm'}\rangle &= \langle\varphi_{Am}|H_{FB}|\varphi_{Cm'}\rangle = 0 \end{aligned} \tag{3.6}$$

for all fermion states $|m\rangle$ and all boson states $|\varphi_{Am}\rangle, |\varphi_{Bm}\rangle, |\varphi_{Cm}\rangle$. For constructional purposes H_{FB} is written as

$$H_{FB} = H_{FB}(0) + \Delta H_{FB}(1) + \Delta H_{FB}(2), \tag{3.7}$$

where $H_{FB}(0), \Delta H_{FB}(1)$ and $\Delta H_{FB}(2)$ must satisfy:

$$\begin{aligned} \langle\varphi_{Am}|H_{FB}|\varphi_{Am'}\rangle &= \langle\varphi_{Am}|H_{FB}(0)|\varphi_{Am'}\rangle, \\ \langle\varphi_{Am}|H_{FB}(0) + \Delta H_{FB}(1)|\varphi_{Cm'}\rangle &= \langle\varphi_{Am}|\Delta H_{FB}(2)|\varphi_{Cm'}\rangle = 0, \\ \langle\varphi_{Am}|H_{FB}(0) + \Delta H_{FB}(2)|\varphi_{Bm'}\rangle &= \langle\varphi_{Am}|\Delta H_{FB}(1)|\varphi_{Bm'}\rangle = 0. \end{aligned} \tag{3.8}$$

The construction of $H_{FB}(0)$ is straightforward and gives (cf. 2.33 - 2.35)

$$H_{FB}(0) = \sum_{\boldsymbol{k},\sigma} \epsilon_{\boldsymbol{k}} n^B_{\boldsymbol{k}\sigma} - \frac{1}{2}{\sum_{\boldsymbol{k},\boldsymbol{q},\sigma}}' V(\boldsymbol{q})\theta(k_F - k)\theta(k_F - |\boldsymbol{k}+\boldsymbol{q}|)$$

$$+ \frac{1}{2} \sum_{\boldsymbol{q},\boldsymbol{k},\boldsymbol{k}',\sigma,\sigma'}'' \left\{ V(\boldsymbol{q}) \left[d^{+}_{-\boldsymbol{q}\sigma'}(-\boldsymbol{k}'\sigma') + d_{\boldsymbol{q}\sigma'}(\boldsymbol{k}'\sigma') \right] \left[d^{+}_{\boldsymbol{q}\sigma}(\boldsymbol{k}\sigma) + d_{-\boldsymbol{q}\sigma}(-\boldsymbol{k}\sigma) \right] \right.$$

$$- V(\boldsymbol{q}+\boldsymbol{k}+\boldsymbol{k}') \left[d^{+}_{-\boldsymbol{q}\sigma'}(-\boldsymbol{k}'\sigma) d^{+}_{\boldsymbol{q}\sigma}(\boldsymbol{k}\sigma') + d_{\boldsymbol{q}\sigma}(\boldsymbol{k}\sigma') d_{-\boldsymbol{q}\sigma'}(-\boldsymbol{k}'\sigma) \right]$$

$$\left. - 2V(\boldsymbol{k}-\boldsymbol{k}') d^{+}_{\boldsymbol{q}\sigma}(\boldsymbol{k}'\sigma') d_{\boldsymbol{q}\sigma}(\boldsymbol{k}\sigma') \right\}. \tag{3.9}$$

The only non-zero matrix elements of the type $\langle \varphi_{Am} | H_{FB}(0) | \varphi_{Cm'} \rangle$ are

(1) those between the states $|\varphi_{Am}\rangle = d^{+}_{\boldsymbol{q}_1\sigma_1}(\boldsymbol{k}_1\sigma_1')|\varphi_{Am-1}\rangle$ and $|\varphi_{Cm'}\rangle = d^{+}_{\boldsymbol{q}_3\sigma_3}(\boldsymbol{k}_3\sigma_3') d^{(+)}_{\boldsymbol{q}_4\sigma_4}(\boldsymbol{k}_4\sigma_4')|\varphi_{Am}\rangle$, where $(\boldsymbol{k}_3\sigma_3') = (\boldsymbol{k}_1\sigma_1')$ or $(\boldsymbol{q}_3\sigma_3) = (\boldsymbol{q}_1 + \boldsymbol{k}_1 - \boldsymbol{k}_3\sigma_1)$ and

(2) those between the states $|\varphi_{Am}\rangle = d^{+}_{\boldsymbol{q}_1\sigma}(\boldsymbol{k}_1\sigma_1') d^{+}_{\boldsymbol{q}_2\sigma_2}(\boldsymbol{k}_2\sigma_2')|\varphi_{Am-2}\rangle$ and $|\varphi_{Cm'}\rangle = d^{+}_{\boldsymbol{q}_3\sigma_3}(\boldsymbol{k}_3\sigma_3') d^{+}_{\boldsymbol{q}_4\sigma_4}(\boldsymbol{k}_4\sigma_4')|\varphi_{Am}\rangle$, where $(\boldsymbol{k}_3\sigma_3') = (\boldsymbol{k}_1\sigma_1')$ and $(\boldsymbol{k}_4\sigma_4') = (\boldsymbol{k}_2\sigma_2)$ or $(\boldsymbol{q}_3\sigma_3) = (\boldsymbol{q}_1 + \boldsymbol{k}_1 - \boldsymbol{k}_3\sigma_1)$ and $(\boldsymbol{k}_4\sigma_4') = (\boldsymbol{k}_2\sigma_2)$ or $(\boldsymbol{q}_3\sigma_3) = (\boldsymbol{q}_1 + \boldsymbol{k}_1 - \boldsymbol{k}_3\sigma_1)$ and $(\boldsymbol{q}_4\sigma_4) = (\boldsymbol{q}_2 + \boldsymbol{k}_2 - \boldsymbol{k}_4\sigma_2)$.

Consequently $\Delta H_{FB}(1)$, which must compensate these matrix-elements, is found to be:

$$\Delta H_{FB}(1) = - \sum_{\boldsymbol{q},\boldsymbol{k},\boldsymbol{k}',\sigma,\sigma'}'' \left\{ \right. [N(\boldsymbol{q},\boldsymbol{k},\sigma,\sigma)$$

$$- \tfrac{1}{2} N(\boldsymbol{q},\boldsymbol{k},\sigma,\sigma) N(-\boldsymbol{q},-\boldsymbol{k}',\sigma',\sigma')] V(\boldsymbol{q}) d_{\boldsymbol{q}\sigma}(\boldsymbol{k}\sigma) d_{-\boldsymbol{q}\sigma'}(-\boldsymbol{k}'\sigma')$$

$$- [N(\boldsymbol{q},\boldsymbol{k},\sigma,\sigma') - \tfrac{1}{2} N(\boldsymbol{q},\boldsymbol{k},\sigma,\sigma') N(-\boldsymbol{q},-\boldsymbol{k}',\sigma',\sigma)] V(\boldsymbol{q}+\boldsymbol{k}+\boldsymbol{k}') d_{\boldsymbol{q}\sigma'}(\boldsymbol{k}\sigma) d_{-\boldsymbol{q}\sigma}(-\boldsymbol{k}'\sigma')$$

$$\left. + N(\boldsymbol{q},\boldsymbol{k},\sigma,\sigma) V(\boldsymbol{q}) d_{\boldsymbol{q}\sigma}(\boldsymbol{k}\sigma) d^{+}_{\boldsymbol{q}\sigma'}(\boldsymbol{k}'\sigma') - N(\boldsymbol{q},\boldsymbol{k},\sigma,\sigma')\, V(\boldsymbol{k}-\boldsymbol{k}') d_{\boldsymbol{q}\sigma'}(\boldsymbol{k}\sigma) d^{+}_{\boldsymbol{q}\sigma'}(\boldsymbol{k}'\sigma) \right\}$$

$$+ c.c. \ , \tag{3.10}$$

where $N(\boldsymbol{q}_1, \boldsymbol{k}_1, \sigma_1, \tau_1) = -d^+_{\boldsymbol{q}_1\tau_1}(\boldsymbol{k}_1\sigma_1) d_{\boldsymbol{q}_1\tau_1}(\boldsymbol{k}_1\sigma_1)$

$$+ \sum_{\boldsymbol{q}', \tau} \left[d^+_{\boldsymbol{q}'\tau}(\boldsymbol{k}_1\sigma_1) d_{\boldsymbol{q}'\tau}(\boldsymbol{k}_1\sigma_1) + d^+_{\boldsymbol{q}_1+\boldsymbol{k}_1-\boldsymbol{q}'\tau_1}(\boldsymbol{q}'\tau) d_{\boldsymbol{q}_1+\boldsymbol{k}_1-\boldsymbol{q}'\tau_1}(\boldsymbol{q}'\tau) \right] .$$

The effect of $\Delta H_{FB}(2)$, which must compensate matrix-elements of the type $\langle \varphi_{Am} | H_{FB}(0) | \varphi_{Bm'} \rangle$, is an additional restriction on the summations in (3.9). This restriction can be phrased as follows: taking into account the term proportional to $d^{(+)}_{-\boldsymbol{q}\sigma'}(-\boldsymbol{k}'\sigma') d^{(+)}_{\boldsymbol{q}\sigma}(\boldsymbol{k}\sigma)$ means discarding the term proportional to $d^{(+)}_{\boldsymbol{q}+\boldsymbol{k}+\boldsymbol{k}'\sigma}(-\boldsymbol{k}'\sigma') d^{(+)}_{-\boldsymbol{q}-\boldsymbol{k}-\boldsymbol{k}'\sigma'}(\boldsymbol{k}\sigma)$. Such a restriction cannot be made mathematically explicit in general. In the present case, however, this problem does not apply as the restriction due to $\Delta H_{FB}(2)$ is already contained in the relatively simple restriction $q < r_s^{1/4} k_F < |\boldsymbol{q} + \boldsymbol{k} + \boldsymbol{k}'|$, i.e.

$$\Delta H_{FB}(2) = 0. \tag{3.11}$$

It should be remarked here that (3.11) does not hold at lower densities, where interaction terms with momentum transfer $q \gtrsim k_F$ become important for the ground state energy and a restriction $q < r_s^{1/4} k_F < |\boldsymbol{q} + \boldsymbol{k} + \boldsymbol{k}'|$ cannot be imposed.

The Hamiltonian H_{FB}, given by (3.7), (3.9), (3.10) and (3.11), includes the full description of a reduced form of the jellium model with the same ground state energy as the jellium model in the high-density limit. In this sense H_{FB} can be considered as a three-dimensional analogue of Tomonaga's Hamiltonian for the one-dimensional electron system.

It is interesting to compare H_{FB} with Sawada's Hamiltonian H_S (3.4), which also leads to the exact ground state energy of the jellium model for $r_s \to 0$. The two Hamiltonians differ strongly from a fundamental point of view. The present Hamiltonian H_{FB} is a boson formulation of the fermion system defined by (3.5) whereas H_S does not include a description of a fermion system at all, i.e. its meaning is unclear.

4. Conclusions

The purpose of the present paper is to describe the interacting electron system in terms of bosons. The present boson formulation consists of an algorithm for the construction of a boson Hamiltonian H_B, which includes a full description of the jellium model at all densities. An explicit construction has been presented for a reduced form of the jellium model with the same ground state energy as the jellium model in the high-density limit. The obtained Hamiltonian H_{FB} has been compared with Sawada's Hamiltonian H_S, which also gives the exact ground state energy of the jellium model for $r_s \to 0$. In contrast with H_{FB} the Sawada Hamiltonian does not describe a fermion system. Consequently a full analysis of the high-density electron system in terms of H_S is questionable from a fundamental point of view. Notably the conclusion cannot be sustained that the elementary excitations of H_S do indeed correspond with the elementary excitations of the jellium model in the high-density limit.

The present boson formulation has not lead to new numerical results nor to a boson Hamiltonian that seems promising for a calculation of the properties of the electron system at lower densities. At first sight the appearing Hamiltonian H_B (2.17) seems an attractive starting-point. For it seems natural to neglect the very complicated term ΔH_B and to diagonalize the bilinear part of $H_B^1 + H_B^2$ while accounting for the remaining terms of $H_B^1 + H_B^2$ by means of a perturbation calculation. However, there is a snake in the grass here. Namely, at lower densities interaction terms with larger momentum transfers get important. This means that a neglect of ΔH_B can no longer be justified. Therefore such a perturbation procedure lacks a satisfactory systematics just as a perturbation calculation starting from Sawada's Hamiltonian, i.e. the results of such a calculation are just as questionable.

Summarizing: the significance of the present boson formulation lies in the fundamental sphere, not in the practical one. The question has been raised and answered in which way the interacting electron system can be described in terms of bosons.

Appendix

Consider the Hamiltonian $\tilde{H}'_F$, which is obtained from $\tilde{H}_F$ (3.1) by taking into account only those interaction terms with momentum transfer $q < q_0 \ll k_F$, where q_0 is some cut-off momentum transfer. In the high-density limit ($r_s \to 0$), the ground state energy of $\tilde{H}'_F$ can be expressed as follows [7] [8]:

$$E_0 = 2N \left[\frac{2.2}{r_s^2} - \frac{0.9}{r_s} + \frac{3}{16\pi^2 r_s^2} \left(\frac{9\pi}{4}\right)^{2/3} \int_{-\infty}^{\infty} du \int_0^{q_0/k_F} 4\pi q^3 dq \right. \left[\ln\left[1 + \frac{\chi(u)}{q^2}\right] - \frac{\chi(u)}{q^2} \right] \Bigg], \tag{A.1}$$

where

$$\chi(u) = \frac{4r_s}{\pi} \left(\frac{4}{9\pi}\right)^{1/3} \left[1 - u \arctan\frac{1}{u}\right]. \tag{A.2}$$

The integral over q can be easily calculated leading to

$$E_0 = 2N \left[\frac{2.2}{r_s^2} - \frac{0.9}{r_s} + \frac{3}{16\pi r_s^2} \left(\frac{9\pi}{4}\right)^{2/3} \int_{-\infty}^{\infty} du \left[\left(\frac{q_0^4}{k_F^4} - \chi^2\right) \ln\left(\chi + \frac{q_0^2}{k_F^2}\right) - \chi \frac{q_0^2}{k_F^2} - \frac{q_0^4}{k_F^4} \ln\frac{q_0^2}{k_F^2} + \chi^2 \ln\chi \right] \right]. \tag{A.3}$$

This result gives the exact ground state energy (3.2) in the limit $r_s \to 0$ provided that $\frac{q_0^2}{k_F^2} \gg \chi_{max}$, where $\chi_{max} = \chi(0) = \frac{4r_s}{\pi} \left(\frac{4}{9\pi}\right)^{1/3}$ is the maximum value of the function χ. This requirement is satisfied by choosing $q_0 = r_s^{1/4} k_F$ as χ_{max} is proportional to r_s.

In order to show that H_F (3.5) leads to the exact ground state energy (3.2) it must be argued now that the additional restriction $|\boldsymbol{q} + \boldsymbol{k} + \boldsymbol{k}'| > r_s^{1/4} k_F$, which is the only difference between H_F and $\tilde{H}'_F$, does not affect E_0 up to order $\ln r_s$, i.e.

$$\lim_{r_s \to 0} \left[\frac{\frac{1}{2N} \left[\langle \varphi_0 | \tilde{H}'_F | \varphi_0 \rangle - \langle \varphi_0 | H_F | \varphi_0 \rangle \right]}{\ln r_s} \right] = 0, \tag{A.4}$$

where $|\varphi_0\rangle$ is the ground state of $\tilde{H}'_F$.

For that purpose the following function is introduced:

$$F_{\sigma\sigma'}(\boldsymbol{q}, \boldsymbol{k}, \boldsymbol{k}') =$$

$$\frac{1}{2} \theta(r_s^{1/4} k_F - q) \theta(k_F - k) \theta(k_F - k') \theta(|\boldsymbol{k} + \boldsymbol{q}| - k_F)\, \theta(|\boldsymbol{k}' + \boldsymbol{q}| - k_F) V(\boldsymbol{q}) \Big[$$

$$\langle \varphi_0 | \left[c^+_{-\boldsymbol{k}'-\boldsymbol{q}\sigma'} c_{-\boldsymbol{k}'\sigma'} + c^+_{\boldsymbol{k}'\sigma'} c_{\boldsymbol{k}'+\boldsymbol{q}\sigma'} \right] \left[c^+_{\boldsymbol{k}+\boldsymbol{q}\sigma} c_{\boldsymbol{k}\sigma} + c^+_{-\boldsymbol{k}\sigma} c_{-\boldsymbol{k}-\boldsymbol{q}\sigma} \right] |\varphi_0\rangle \Big]. \tag{A.5}$$

Using (3.1) together with the definition of $\tilde{H}'_F$ and using (3.2) and (3.5) it appears that in the limit $r_s \to 0$:

$$\sum_{\boldsymbol{k}, \boldsymbol{k}', \boldsymbol{q}, \sigma, \sigma'}{}' F_{\sigma\sigma'}(\boldsymbol{q}, \boldsymbol{k}, \boldsymbol{k}') = 2N \left(0.0622 \ln r_s \right), \tag{A.6}$$

$$\sum_{\boldsymbol{k}, \boldsymbol{k}', \boldsymbol{q}, \sigma, \sigma'}{}' \theta(r_s^{1/4} k_F - |\boldsymbol{k} + \boldsymbol{k}' + \boldsymbol{q}|) F_{\sigma\sigma'}(\boldsymbol{q}, \boldsymbol{k}, \boldsymbol{k}') = \langle \varphi_0 | \tilde{H}'_F | \varphi_0 \rangle - \langle \varphi_0 | H_F | \varphi_0 \rangle.$$

Consequently $\tilde{H}'_F$ and H_F have the same ground state energy in the high-density limit if

$$\lim_{r_s \to 0} \left[\frac{\sum_{\boldsymbol{k}, \boldsymbol{k}', \boldsymbol{q}, \sigma, \sigma'}{}' \theta(r_s^{1/4} k_F - |\boldsymbol{k} + \boldsymbol{k}' + \boldsymbol{q}|) F_{\sigma\sigma'}(\boldsymbol{q}, \boldsymbol{k}, \boldsymbol{k}')}{\sum_{\boldsymbol{k}, \boldsymbol{k}', \boldsymbol{q}, \sigma, \sigma'}{}' F_{\sigma\sigma'}(\boldsymbol{q}, \boldsymbol{k}, \boldsymbol{k}')} \right] = 0. \tag{A.7}$$

The denominator in the left hand side of (A.7) can be expressed as follows in the limit

$r_s \to 0$:

$$\sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q},\sigma,\sigma'}{}' F_{\sigma\sigma'}(\boldsymbol{q},\boldsymbol{k},\boldsymbol{k}') = C\int_0^{q_0} q^2 dq \int_0^1 dx \int_0^1 dy \Big[\int_{k_F - qx}^{k_F} k^2 dk \int_{k_F - qy}^{k_F} k'^2 dk' \int_0^{2\pi} d\varphi F_{\sigma\sigma'}(q,k,k',x,y)\Big], \tag{A.8}$$

where x, y and φ are defined by

$$\begin{aligned} \boldsymbol{k}\cdot\boldsymbol{q} &= kqx, \\ \boldsymbol{k}'\cdot\boldsymbol{q} &= k'qy, \\ \boldsymbol{k}\cdot\boldsymbol{k}' &= kk'\Big[xy - \sqrt{1-x^2}\sqrt{1-y^2}\cos\varphi\Big], \end{aligned} \tag{A.9}$$

$q_0 = k_F\, r_s^{1/4}$ and C is some constant. It should be remarked that the function F is independent of φ. The reason being that each function value $F_{\sigma\sigma'}(\boldsymbol{q},\boldsymbol{k},\boldsymbol{k}')$ can be interpreted as a sum over ring diagrams. The numerator in (A.7) is also of the form (A.8), but now the following restriction must be imposed:

$$q^2 + k^2 + k'^2 + 2qkx + 2qk'y + 2kk'\Big[xy - \sqrt{1-x^2}\sqrt{1-y^2}\cos\varphi\Big] < k_F^2 r_s^{1/2}. \tag{A.10}$$

It can easily be checked that for $r_s \to 0$, where it holds that $k - k_F$, $k' - k_F$ and q are of the order of $r_s^{1/4}\, k_F$ or smaller, the restriction (A.10) leads to:

$$1 - \frac{1}{2}\varepsilon^2 \le \cos\varphi \le 1 \tag{A.11}$$

i.e

$$0 \le \varphi \le \varepsilon, \tag{A.12}$$

where ε is of the order of $r_s^{1/4}$. From (A.8) and (A.12) it follows directly that the requirement (A.7) is satisfied, i.e. $\tilde{H}'_F$ and H_F have the same ground state energy in the high-density limit.

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Samenvatting

Dit proefschrift heeft als onderwerp: de formulering van het jellium model in termen van bosonen.

Het jellium model bestaat uit wisselwerkende elektronen, die bewegen tegen een homogene achtergrond van positieve lading. De betreffende wisselwerking is de Coulomb wisselwerking. Het systeem als geheel is neutraal, d.w.z. de totale lading van de elektronen heft de positieve lading van de homogene achtergrond op. Het jellium model kan gezien worden als een vereenvoudigd model voor een metaal, waarbij het rooster van de metaalionen is vervangen door de homogene achtergrond van positieve lading. De bestudering van het jellium model heeft bijgedragen tot inzicht in het gedrag van elektronen in metalen.

Het jellium model is nog dusdanig gecompliceerd dat alleen exacte oplossingen bekend zijn voor zeer lage en zeer hoge elektronendichtheid. Eén van de methoden, die tot deze exacte oplossingen leiden, is het formuleren van het jellium model in termen van bosonen. De bestaande boson formuleringen doen echter onvoldoende recht aan het fermion karakter van het jellium model. Dit roept de fundamentele vraag op naar hun betekenis. In dit proefschrift komt deze vraag aan de orde en worden andere boson formuleringen gepresenteerd.

Het proefschrift bestaat uit twee delen. Deel I behandelt het jellium model in de limiet van zeer lage dichtheid. In deze limiet gedragen de elektronen zich min of meer als klassieke onderscheidbare deeltjes. De grondtoestand van het klassieke jellium model blijkt een rooster van stilstaande elektronen te zijn (hoofdstuk 2). Wigner heeft laten zien,

dat de grondtoestand van het quantummechanische jellium model bij zeer lage dichtheid nog steeds kan worden voorgesteld door een rooster. Echter nu staan de elektronen niet stil, maar trillen ze om de roosterplaatsen. In de theorie van Wigner zijn de trillingen van de elektronen niet aan elkaar gekoppeld met als gevolg dat voor de trillingsenergie van de elektronen in de grondtoestand een te hoge waarde wordt gevonden. Carr heeft de theorie van Wigner verbeterd door deze trillingen te koppelen. In de theorie van Carr wordt de exacte trillingsenergie voor zeer lage elektronendichtheid gevonden door de Hamiltoniaan van het jellium model te ontwikkelen in de uitwijkingen van de elektronen uit hun evenwichtsposities in het rooster en het resultaat m.b.v. een lineaire transformatie te schrijven als een boson Hamiltoniaan. Deze semi-klassieke procedure heeft echter tot gevolg dat het fermion-karakter van het jellium model volledig verloren gaat.

In deel I wordt de semi-klassieke aanpak vervangen door een volledig quantummechanische methode. De resultaten van Wigner blijken overeen te komen met die van een Hartree-Fock theorie, waarbij de grondtoestand een Slater-determinant is bestaande uit de grondtoestandsfunkties van harmonische oscillatoren, die gelokaliseerd zijn op de roosterposities van het Wigner rooster (hoofdstuk 3). In de theorie van Wigner wordt de overlapping van twee funkties op verschillende roosterplaatsen verwaarloosd. In de Hartree-Fock theorie kan deze overlapping, die aanleiding geeft tot het voor fermionen karakteristieke "exchange-effect" op relatief eenvoudige wijze worden meegenomen. Het blijkt dan dat voor lage elektronendichtheid een ferromagnetisch rooster de voorkeur verdient boven een anti-ferromagnetisch rooster. De resultaten van Carr worden verkregen door de elektron-elektron correlatie mee te nemen. Dit gebeurt in drie stappen (hoofdstuk 4). Eerst worden de eigentoestanden van het jellium model geschreven als lineaire combinaties van alle mogelijke Slater-determinanten van eigenfuncties van harmonische oscillatoren, die gelokaliseerd zijn op de roosterposities van het Wigner-rooster. Vervolgens wordt een effectieve Hamiltoniaan ingevoerd, die dezelfde eigenwaarden heeft als de oorspronkelijke Hamiltoniaan van het jellium model, wanneer het "exchange-effect" wordt verwaarloosd. Door tenslotte gebruik te maken van een transformatie, die een direkt verband geeft tussen

fermionen en bosonen, wordt een boson Hamiltoniaan verkregen, die het jellium model bij zeer lage elektronendichtheid volledig beschrijft. De zo verkregen boson formulering wordt gebruikt om het effect van een magnetisch veld op het jellium model te bestuderen (hoofdstuk 5). Met name wordt nagegaan of een Meissner-Ochsenfeld effect, zoals dat bij supergeleiders voorkomt, in het jellium model met zeer lage elektronendichtheid kan optreden. Dit blijkt niet het geval te zijn.

Deel II van het proefschrift behandelt het jellium model in de limiet van zeer hoge dichtheid. In deze limiet wordt het model meestal bestudeerd m.b.v. storingstheorie, waarbij het vrije elektron model van Sommerfeld wordt gebruikt als ongestoord systeem. Een dergelijke storingstheorie leidt reeds in tweede orde tot een divergentie in de grondtoestandsenergie als gevolg van de lange dracht van de Coulomb wisselwerking. Gell-Mann en Brueckner hebben dit probleem omzeild door de meest divergente storingstermen, die kunnen worden voorgesteld door zogenaamde ringdiagrammen, op een bepaalde wijze te sommeren. Hun berekening leidt tot de exacte grondtoestandsenergie in de hoge dichtheidslimiet, maar is op zichzelf niet gerechtvaardigd. Sawada heeft de grondtoestandsenergie berekend door eerst alle bijdragen van de Coulomb wisselwerking, die niet leiden tot ringdiagrammen, uit het jellium model te verwijderen en daarna het overblijvende deel van de Hamiltoniaan als een exact oplosbare boson Hamiltoniaan te schrijven zonder zich om de juiste fermion-commutatierelaties te bekommeren. Sawada's boson formulering kan gerechtvaardigd worden vanuit het standpunt van storingstheorie, aangezien het niet gebruiken van de juiste fermion-commutatierelaties in de limiet van hoge dichtheid een verwaarloosbaar effect heeft op de grondtoestandsenergie, vergeleken met de bijdrage van de ringdiagrammen. De methode heeft echter tot gevolg dat de verkregen boson Hamiltoniaan in het geheel geen systeem van fermionen beschrijft. De betekenis van deze Hamiltoniaan is derhalve onduidelijk.

In deel II wordt een algorithme gegeven voor de constructie van een boson Hamiltoniaan, die de volledige beschrijving van het jellium model bevat voor elke elektronendichtheid (hoofdstuk 2). De boson Hamiltoniaan wordt zodanig geconstrueerd, dat zijn

matrixrepresentatie op een deelverzameling van boson toestanden, die één op één correspondeert met de volledige verzameling van fermion toestanden, volledig identiek is aan de matrixrepresentatie van het jellium model op de genoemde verzameling van fermion toestanden. Voorts wordt gezorgd dat de matrixelementen van de boson Hamiltoniaan tussen boson toestanden, die deel uitmaken van de genoemde deelverzameling, en de overige boson toestanden nul zijn. De eigenwaarden van het jellium model vormen dan een deelverzameling van de eigenwaarden van deze boson Hamiltoniaan. In het algemeen kan de constructie van deze boson Hamiltoniaan niet expliciet worden uitgevoerd. Dit lukt echter wel in het speciale geval van een wisselwerkend fermion systeem, dat uit het jellium model is verkregen door het verwijderen van die bijdragen van de Coulomb wisselwerking, die bij zeer hoge elektronendichtheid een verwaarloosbaar effect hebben op de grondtoestandsenergie (hoofdstuk 3). Het resultaat van deze constructie is een boson Hamiltoniaan, die de volledige beschrijving bevat van een gereduceerde vorm van het jellium model. Dit gekortwiekte model heeft dezelfde grondtoestandsenergie als het jellium model bij zeer hoge elektronendichtheid.

Curriculum Vitae

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1980:	Eindexamen gymnasium β aan het Collegium Marianum te Venlo.
1983:	Kandidaatsexamens natuurkunde en sterrenkunde aan de Katholieke Universiteit Nijmegen (KUN).
1986:	Doctoraal examen theoretische natuurkunde met bijvak sterrenkunde aan de KUN.
	Afstudeerwerk verricht o.l.v. Prof.Dr. G. Vertogen.
	Titel van de doctoraalscriptie: Theorie van supergeleiding.
1984-1986:	Opleiding tot eerstegraads leraar natuurkunde aan de KUN.
1986-1987:	Wetenschappelijk medewerker in dienst van de stichting Fundamenteel Onderzoek der Materie (FOM) bij de groep Electronenstructuur van Materialen (ESM) aan de KUN, o.l.v. Prof.Dr. A.G.M. Janner en Dr. R.A. de Groot.
1987-1990:	Assistent in Opleiding (AIO) in dienst van de KUN.
	Promotie onderzoek verricht o.l.v. Prof.Dr. G. Vertogen.
1990-heden:	Leraar natuurkunde aan "De Springbron", scholengemeenschap voor MAVO-HAVO-Atheneum te Epe.

Stellingen

behorende bij het proefschrift

Bosons in Jellium

1 Een bewijs voor de door B C S gebruikte aanname, dat de elektron-phonon wisselwerking leidt tot een elektron elektron attractie, die sterker is dan de Coulomb-repulsie, is nog nooit geleverd

J Bardeen, L N Cooper en J R Schrieffer Phys Rev **108**, *1175 (1957)*

D Pines Phys Rev **109**, *280 (1958)*

P Morel en P W Anderson Phys Rev **125**, *1263 (1962)*

F W Pijpers en G Vertogen J Physique **43**, *97 (1982)*

2 De oplossing van het Tomonaga model zoals gepresenteerd door Mahan is niet correct Zelfs na enige ten onrechte gebruikte benaderingen zijn de gevonden excitaties nog niet elementair In werkelijkheid is het Tomonaga model onder bepaalde voorwaarden exact oplosbaar

G D Mahan Many-particle physics, Plenum Press, New York (1981)

S Tomonaga Prog Theor Phys **5**, *544 (1950)*

3. Het al dan niet bestaan van de superstroom in een model voor supergeleiding moet worden aangetoond door beide macroscopische vergelijkingen van London volgens de regels van de quantummechanica af te leiden De gebruikelijke "klassieke" argumenten, zoals het optreden van deeltjesparen, zijn volstrekt onvoldoende

4 De uitspraak "over smaak valt niet te twisten" wordt vaak gebezigd waar men bedoelt te zeggen "Objectieve criteria ter beoordeling van de kwaliteit van kunstuitingen bestaan niet" Het eerste is zonder twijfel waar, het tweede is daarentegen niet waar

5 De vergelijking, die Pais trekt tussen de ontwikkeling van speciale naar algemene relativiteitstheorie en die van Mozarts muziek naar Beethovens strijkkwartet opus 135, gaat volledig mank omdat ze geen rekening houdt met datgene, waarin de fysica fundamenteel verschilt van de muziek de falsifieerbaarheid van hetgeen ze te zeggen heeft

6. De tendens van het VWO-examen natuurkunde, een verbreding van de examenstof ten koste van vooral mathematische verdieping, gaat lijnrecht in tegen de historische ontwikkeling van de fysica sinds de zeventiende eeuw. Deze kenmerkt zich immers door toenemende specialisering en mathematisering. Van het WEN-examenprogramma valt dan ook niet te verwachten dat het de aansluiting van het VWO op het universitair natuurkundeonderwijs zal bevorderen.

7. Wanneer beleidsmakers in het onderwijs geen rekening houden met het belang van de onderwijsgevenden handelen zij juist niet in het belang van hen, die het onderwijs ontvangen. Hun beleid is in dat geval inconsistent!

8. De reeds door Thomas van Aquino gepostuleerde harmonie tussen geloof en wetenschap kan door geen enkel resultaat van de wetenschap worden verstoord aangezien de geopenbaarde waarheid niet voor weerlegging door de rede vatbaar is.

9. Dat het naïeve beeld van de Newtoniaanse wereldmachine en de daarmee gepaard gaande theologische en filosofische consequenties na drie eeuwen zelfs door een aantal vooraanstaande fysici, onder wie Hawking en Davies, nog steeds wordt aangehangen toont aan hoe noodzakelijk het is, dat voor natuurkundestudenten tenminste een inleidende cursus in de filosofie en/of de theologie verplicht wordt gesteld.

   S. Hawking: Het heelal, Bert Bakker, Amsterdam (1988).

   P. Davies: God and the new physics, Penguin, London (1983).

10. Een natuurwetenschapper, die niet in het bestaan van een God gelooft, moet wel een gespleten persoonlijkheid bezitten.

    Vrij naar S. van der Meer: Interview in NRC-Handelsblad, 18-4-1987.

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